



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 09:00 AM EDT

PDB ID : 5WFS / pdb_00005wfs
EMDB ID : EMD-8829
Title : 70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C4)
Authors : Fislage, M.; Frank, J.
Deposited on : 2017-07-12
Resolution : 3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

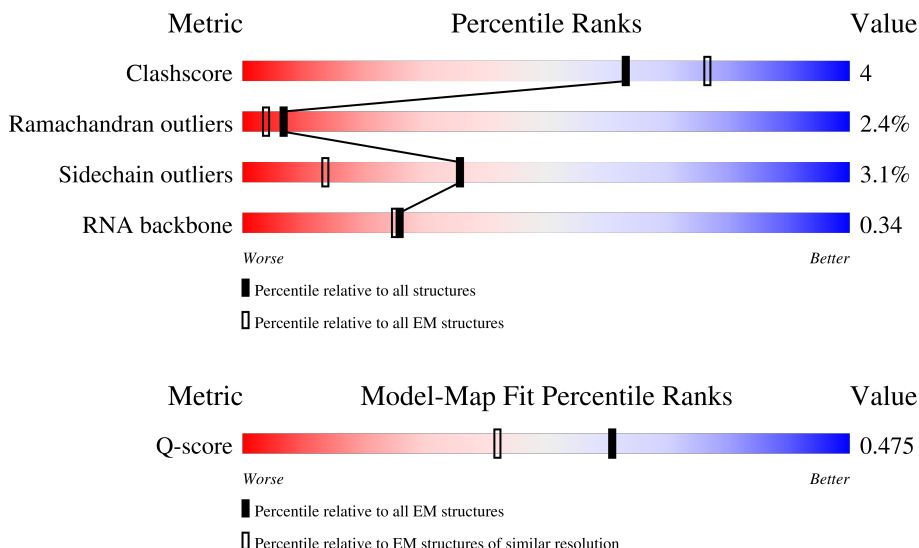
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



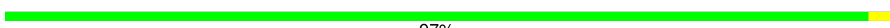
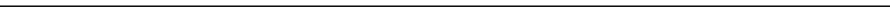
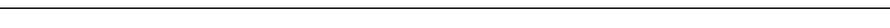
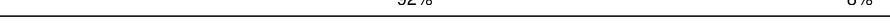
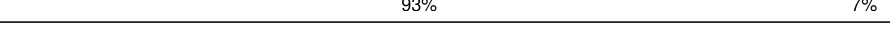
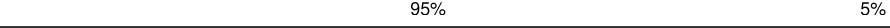
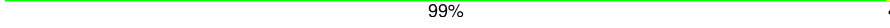
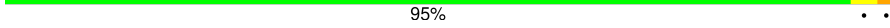
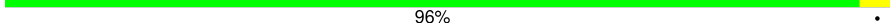
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	271	

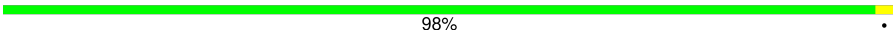
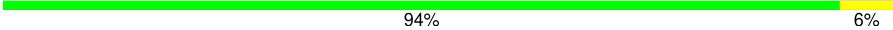
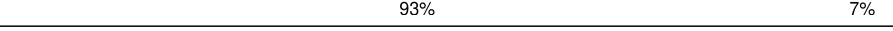
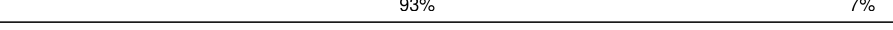
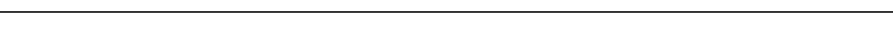
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Mol	Chain	Length	Quality of chain
4	D	208	 91% 8%
5	E	200	 90% 9%
6	F	177	 90% 8% .
7	G	174	 97% . .
8	H	149	 10% 91% 8% .
9	I	141	 24% 84% 15% .
10	J	141	 91% 8% .
11	K	122	 89% 11%
12	L	143	 87% 10% .
13	M	136	 93% 7%
14	N	119	 88% 12%
15	O	116	 94% 6%
16	P	114	 90% 9% .
17	Q	115	 90% 10%
18	R	102	 87% 13%
19	S	109	 92% 8%
20	T	92	 90% 10%
21	U	102	 93% 7%
22	V	92	 91% 9%
23	W	75	 95% 5%
24	X	77	 99% .
25	Y	60	 95% . .
26	Z	56	 96% .
27	0	55	 91% 7% .
28	1	51	 100%

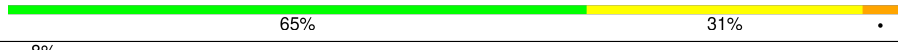
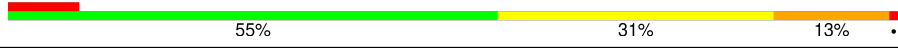
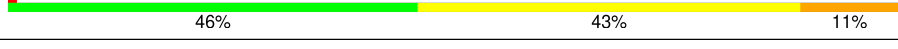
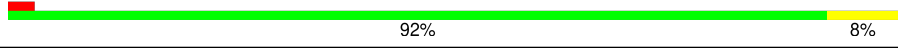
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Mol	Chain	Length	Quality of chain
29	2	45	 84% 16%
30	3	64	 98% .
31	4	38	 89% 11%
32	5	131	 89% 9% .
33	6	66	 92% 8%
34	a	1540	 55% 35% 9% .
35	b	218	 94% 6%
36	c	206	 92% 6% .
37	d	205	 93% 7%
38	e	157	 83% 16% .
39	f	100	 87% 9% .
40	g	151	 89% 10% .
41	h	129	 88% 12%
42	i	127	 93% 7% .
43	j	98	 91% 8% .
44	k	116	 93% 7%
45	l	121	 89% 10% .
46	m	115	 91% 8% .
47	n	101	 86% 13% .
48	o	88	 91% 8% .
49	p	82	 87% 13%
50	q	80	 84% 15% .
51	r	65	 80% 18% .
52	s	79	 91% 9%
53	t	85	 91% 9%

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Mol	Chain	Length	Quality of chain
54	u	65	
55	v	77	
55	w	77	
56	x	12	
57	y	76	
58	z	393	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	A	2030	-	-	X	-
63	GTP	z	402	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155100 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2900	Total	C	N	O	P	0	0
			62277	27788	11459	20130	2900		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 216643
A	1723	G	A	conflict	GB 216643
A	1847	G	A	conflict	GB 216643

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1199817771

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1557	974	287	293	3		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	200	Total	C	N	O	S	0	0
			1544	969	282	289	4		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	115	Total	C	N	O	0	0
			933	595	190	148		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	92	Total	C	N	O	S	0	0
			739	471	135	131	2		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total	C	N	O	S	0	0
			572	355	116	100	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total	C	N	O	S	0	0
			494	305	96	91	2		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	51	Total	C	N	O	S	0	0
			417	269	76	72			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	1	0
			1164	724	221	213	6		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			810	502	165	140	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP B7MCS2

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0
55	w	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	43	84	12		

- Molecule 57 is a RNA chain called Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

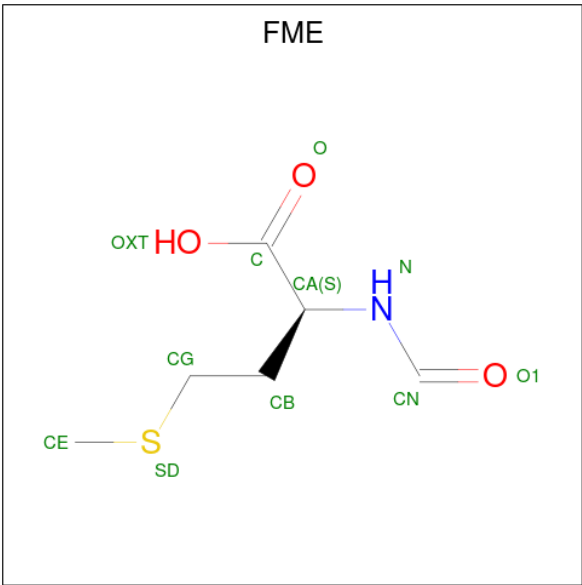
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	522	581	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	84	ALA	HIS	engineered mutation	UNP A7ZUJ2

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
59	A	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	1011	Total	Mg	0
			1011	1011	
60	B	37	Total	Mg	0
			37	37	
60	C	1	Total	Mg	0
			1	1	
60	D	2	Total	Mg	0
			2	2	
60	E	1	Total	Mg	0
			1	1	
60	M	2	Total	Mg	0
			2	2	
60	N	1	Total	Mg	0
			1	1	
60	Q	1	Total	Mg	0
			1	1	
60	T	1	Total	Mg	0
			1	1	
60	W	1	Total	Mg	0
			1	1	
60	0	3	Total	Mg	0
			3	3	

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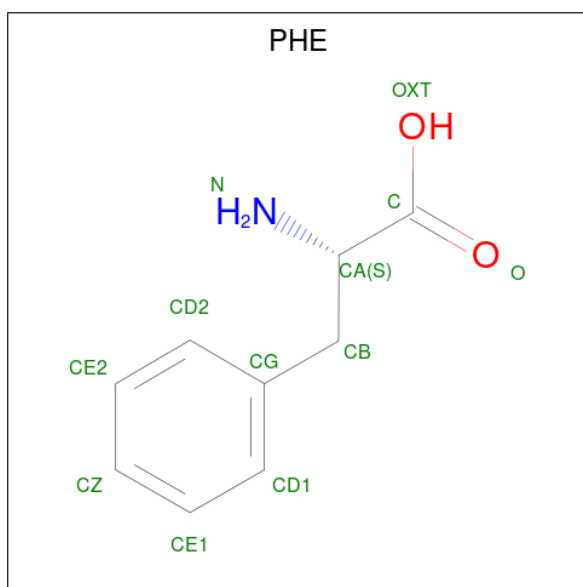
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	2	1	Total 1	Mg 1	0
60	a	392	Total 392	Mg 392	0
60	d	1	Total 1	Mg 1	0
60	e	1	Total 1	Mg 1	0
60	i	1	Total 1	Mg 1	0
60	u	1	Total 1	Mg 1	0
60	v	6	Total 6	Mg 6	0
60	w	2	Total 2	Mg 2	0
60	x	1	Total 1	Mg 1	0
60	y	2	Total 2	Mg 2	0
60	z	2	Total 2	Mg 2	0

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

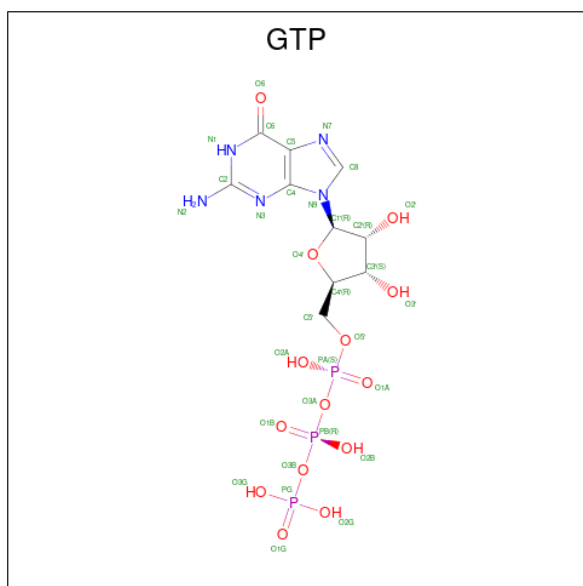
Mol	Chain	Residues	Atoms		AltConf
61	A	6	Total 6	K 6	0
61	a	1	Total 1	K 1	0

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				AltConf
62	z	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	AltConf
64	A	828	Total O 828 828	0
64	B	29	Total O 29 29	0
64	C	5	Total O 5 5	0
64	D	6	Total O 6 6	0
64	E	5	Total O 5 5	0
64	J	4	Total O 4 4	0
64	L	5	Total O 5 5	0
64	N	1	Total O 1 1	0
64	O	1	Total O 1 1	0
64	Q	3	Total O 3 3	0
64	R	1	Total O 1 1	0
64	S	3	Total O 3 3	0
64	W	2	Total O 2 2	0
64	X	3	Total O 3 3	0
64	Y	1	Total O 1 1	0
64	0	2	Total O 2 2	0
64	1	1	Total O 1 1	0
64	2	2	Total O 2 2	0
64	3	1	Total O 1 1	0
64	a	253	Total O 253 253	0
64	c	1	Total O 1 1	0
64	i	1	Total O 1 1	0

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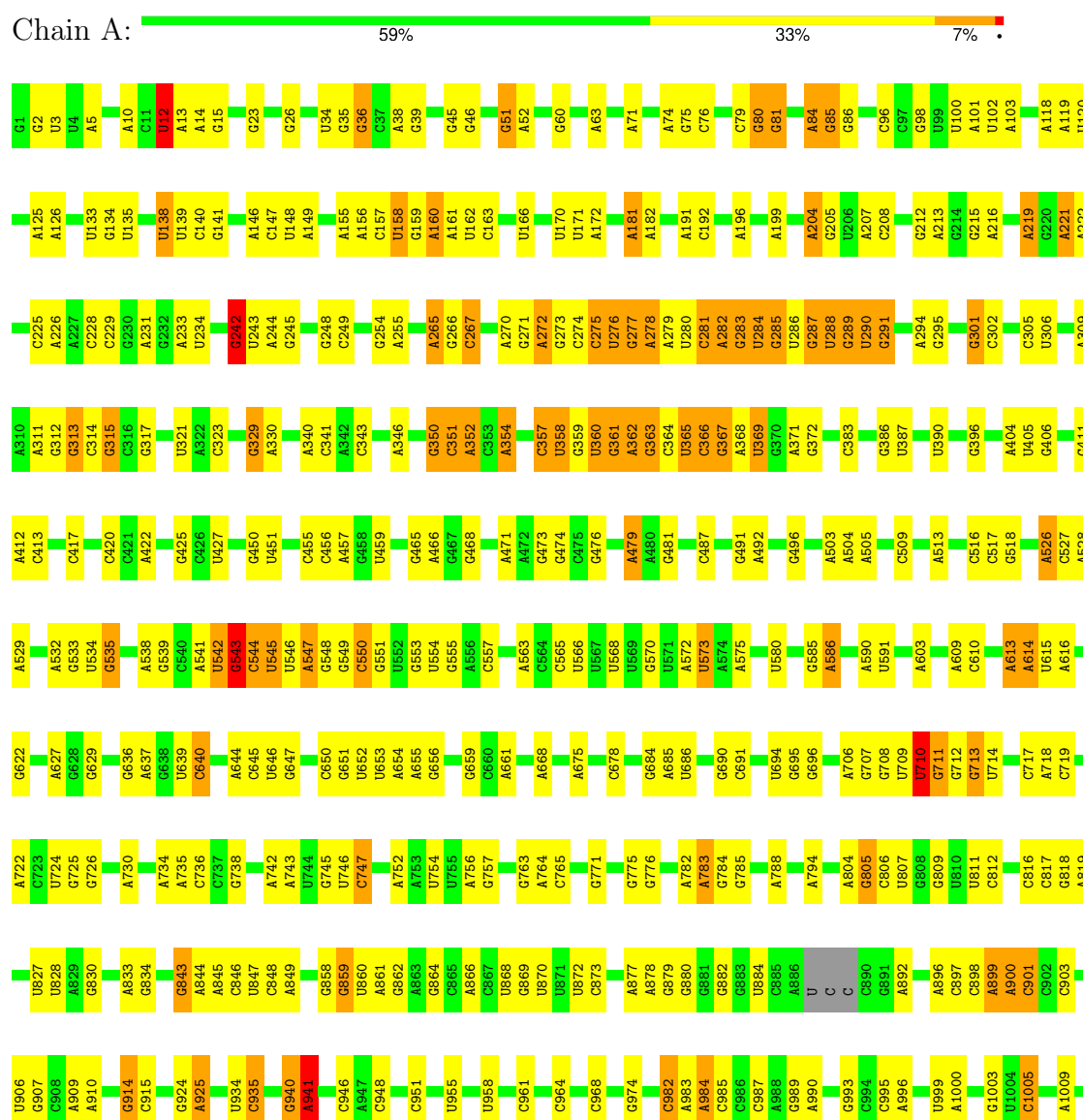
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Mol	Chain	Residues	Atoms		AltConf
64	j	1	Total 1	O 1	0
64	l	2	Total 2	O 2	0
64	m	1	Total 1	O 1	0
64	o	1	Total 1	O 1	0
64	q	1	Total 1	O 1	0
64	s	3	Total 3	O 3	0
64	u	1	Total 1	O 1	0
64	v	3	Total 3	O 3	0
64	w	1	Total 1	O 1	0
64	x	1	Total 1	O 1	0
64	y	2	Total 2	O 2	0

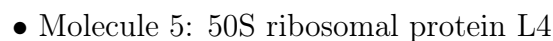
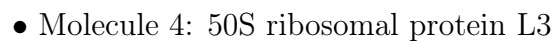
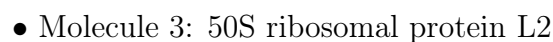
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 23S rRNA



G2315	U2202	A2094	G2004	G1907	A1808	U1693	A1571	A1490	G1288	G1154	A1077	U1012
G2319	U2203	A2095	A2013	U1911	A1809	G1694	A1572	G1491	C1289	A1165	U1076	C1013
G2320	U2204	A2096	A2096	U1912	G1810	G1695	U1578	G1492	C1297	A1084	C1079	A1014
U2321	U2098	U2098	U2016	A1913	U1812	U1579	A1579	G1493	G1300	A1085	U1019	U1015
A2322	U2099	U2099	A2020	C1914	G1816	G1703	A1580	A1494	A1301	A1086	A1020	A1021
G2323	G2100	G2100	A2021	A1916	G1817	G1715	A1581	A1495	A1306	A1087	G1022	G1022
U2324	G2101	G2101	C2022	U1917	G1818	U1716	A1582	A1496	C1306	A1088	A1023	U1023
G2325	G2102	G2102	C2023	U1918	A1819	A1717	A1583	G1418	A1301	A1089	G1024	G1024
A2326	U2106	U2106	U2024	U1923	G1830	G1721	C1585	A1502	C1306	A1090	G1025	G1025
A2327	G2107	G2107	C2025	U1924	G1831	A1722	U1589	A1503	A1321	A1095	A1027	A1027
U2328	A2108	A2108	U2026	C1925	G1832	G1723	A1590	A1504	A1097	A1096	A1028	A1028
G2330	U2109	U2109	G2027	U1926	C1833	G1724	A1591	A1505	A1178	U1101	U1032	U1032
G2331	G2223	G2223	U2028	U1927	G1834	C1725	A1592	A1506	U1180	U1102	U1033	U1033
G2332	U2110	U2110	A2029	A1928	U1835	G1726	C1592	A1507	U1181	A1103	G1034	G1034
A2333	G2224	G2224	A2030	G1929	G1836	A1727	U1599	A1508	C1330	A1104	U1035	U1035
G2334	G2225	G2225	A2031	G1930	G1837	C1728	C1600	G1510	G1343	U1183	U1036	U1036
A2336	U2113	U2113	G2032	U1931	G1839	U1729	A1603	G1514	U1344	G1190	G1106	A1039
G2337	U2118	U2118	A2033	A1932	G1842	U1730	C1604	A1515	G1345	G1195	U1108	A1040
G2345	A2119	A2119	C2036	U1933	G1847	C1731	C1607	G1519	G1346	U1109	G1041	G1041
A2346	G2120	G2120	A2037	A1936	U1851	U1733	A1608	A1522	C1350	U1110	G1042	G1042
C2347	G2121	G2121	G2038	A1937	U1852	C1732	A1609	U1523	C1351	A1111	C1043	C1043
G2350	G2127	G2127	U2039	U1938	A1853	G1735	A1610	G1524	U1203	G1112	U1113	U1113
C2351	U2131	U2131	A2042	U1940	G1857	G1738	C1611	G1529	A1204	A1113	C1044	C1044
G2352	U2132	U2132	C2043	A1941	A1858	A1739	G1612	G1538	A1205	C1114	A1046	A1046
A2353	G2133	G2133	G2049	C1942	G1859	G1740	A1614	G1539	U1211	G1115	G1047	G1047
U2356	A2134	A2134	C2050	U1943	G1863	G1750	G1615	U1540	G1361	G1116	A1048	A1048
G2357	G2141	G2141	A2051	G1945	G1866	A1754	C1617	G1541	C1362	C1117	C1049	C1049
G2361	C2145	C2145	C2055	U1955	A1867	C1764	A1618	U1542	A1230	U1118	A1050	A1050
A2362	A2146	A2146	G2056	U1962	G1867	U1764	G1619	G1543	U1231	G1119	G1051	G1051
G2373	G2157	G2157	A2059	U1963	U1870	A1773	G1622	U1544	G1236	C1121	C1052	C1052
A2378	G2162	G2162	A2060	G1964	A1871	G1776	G1642	A1545	U1240	G1124	A1054	A1054
G2383	A2163	A2163	G2061	C1965	A1872	U1779	C1644	U1546	U1246	G1125	G1055	G1055
C2385	C2164	C2164	A2062	G1966	G1873	U1780	U1647	U1547	A1247	A1129	U1056	U1056
U2391	U2291	U2291	C2064	G1967	G1874	A1781	U1648	A1548	G1248	G1130	U1057	U1057
U2292	U2292	U2292	G2067	A1969	A1876	U1782	U1649	U1549	U1249	G1131	U1058	U1058
G2293	U2170	U2170	U2068	U1970	G1877	U1783	A1650	U1550	C1386	U1132	U1060	U1060
G2294	A2171	A2171	A2069	G1972	G1878	A1784	G1651	G1475	A1387	C1135	U1061	U1061
C2295	U2172	U2172	A2070	U1971	U1879	U1785	U1654	U1476	U1250	C1136	G1062	G1062
A2296	A2173	A2173	A2071	U1976	U1880	A1786	G1654	A1477	A1253	G1139	G1063	G1063
G2297	G2186	G2186	C2072	U1976	C1881	A1791	A1654	G1478	A1254	U1140	A1064	A1064
A2298	U2187	U2187	C2073	U1982	G1884	G1792	A1654	U1479	U1255	U1065	U1066	U1066
U2302	U2188	U2188	U2074	U1982	A1885	C1793	A1654	G1480	G1256	A1141	A1067	A1067
U2303	U2189	U2189	U2075	U1991	A1885	A1794	A1668	U1558	U1394	A1142	G1068	G1068
U2304	G2306	G2306	U2076	G1992	A1890	C1795	A1668	U1559	A1395	A1143	A1069	A1069
A2405	U2190	U2190	A2077	U1993	A1890	U1796	A1672	U1560	U1396	A1144	A1070	A1070
G2406	U2191	U2191	G2077	U1993	G1896	U1797	G1673	U1563	U1397	G1271	G1071	G1071
A2407	G2307	G2307	C2078	U1993	G1896	G1799	G1674	C1565	C1399	A1268	C1072	C1072
U2408	U2193	U2193	U2079	C1997	G1902	C1800	C1675	U1566	A1403	A1272	A1073	A1073
G2409	A2309	A2309	A2080	A1998	C1902	A1801	C1675	U1567	G1407	U1273	G1074	G1074
G2410	C2311	C2311	U2092	C2000	C1905	A1802	A1678	A1569	A1151	A1287	C1075	C1075
			G2093		G1906		A1679	A1570	G1408			



Chain E:  90% 9%

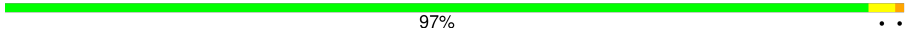


- Molecule 6: 50S ribosomal protein L5

Chain F:  90% 8%

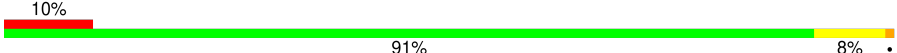


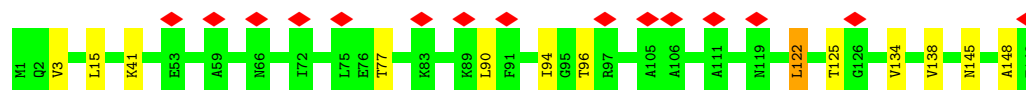
- Molecule 7: 50S ribosomal protein L6

Chain G:  97%



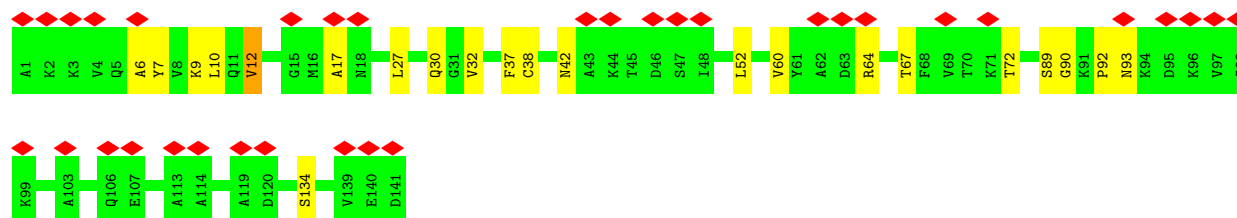
- Molecule 8: 50S ribosomal protein L9

Chain H:  10% 91% 8%



- Molecule 9: 50S ribosomal protein L11

Chain I:  24% 84% 15%



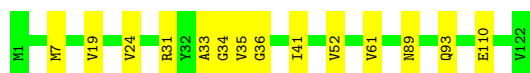
- Molecule 10: 50S ribosomal protein L13

Chain J:  91% 8%

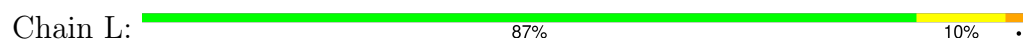


- Molecule 11: 50S ribosomal protein L14

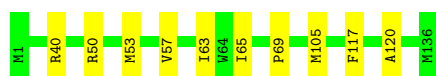
Chain K:  89% 11%



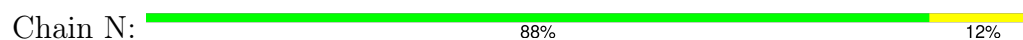
- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



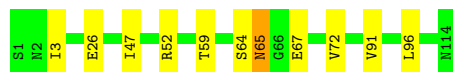
- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19



- Molecule 17: 50S ribosomal protein L20

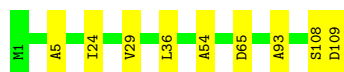


- Molecule 18: 50S ribosomal protein L21





- Molecule 19: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L29





- Molecule 26: 50S ribosomal protein L30

Chain Z: 96%



- Molecule 27: 50S ribosomal protein L32

Chain 0: 91% 7%



- Molecule 28: 50S ribosomal protein L33

Chain 1: 100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L34

Chain 2: 84% 16%



- Molecule 30: 50S ribosomal protein L35

Chain 3: 98%



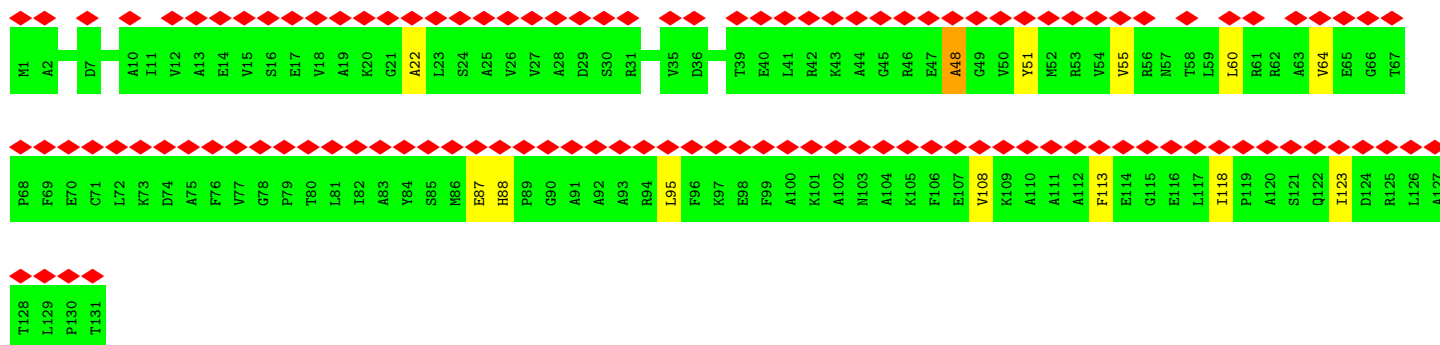
- Molecule 31: 50S ribosomal protein L36 1

Chain 4: 89% 11%



- Molecule 32: 50S ribosomal protein L10

Chain 5: 89% 90% 9%



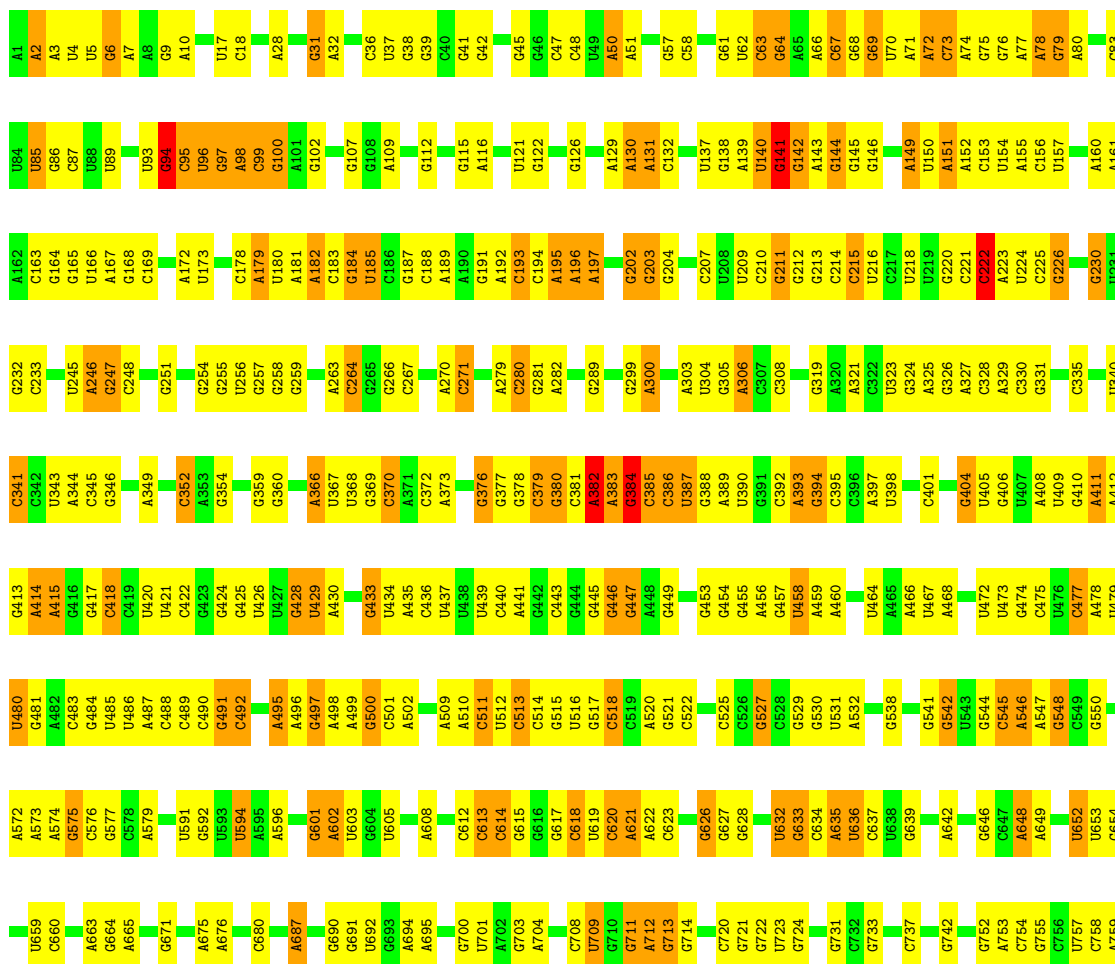
- Molecule 33: 50S ribosomal protein L31

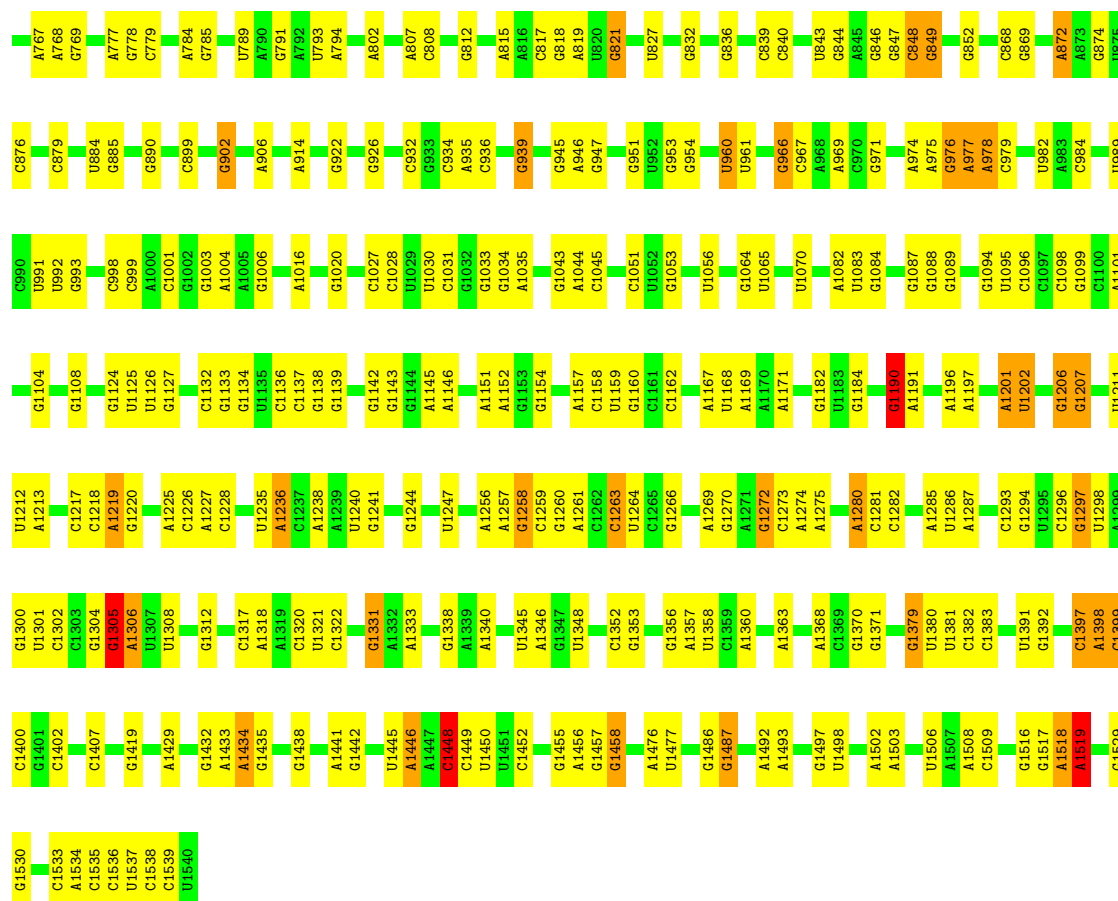
Chain 6:



- Molecule 34: 16S rRNA

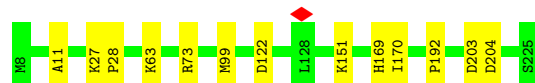
Chain a:





- Molecule 35: 30S ribosomal protein S2

Chain b: 94% 6%



- Molecule 36: 30S ribosomal protein S3

Chain c: 92% 6%



- Molecule 37: 30S ribosomal protein S4

Chain d: 93% 7%



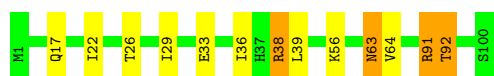
- Molecule 38: 30S ribosomal protein S5

Chain e:  83% 16%



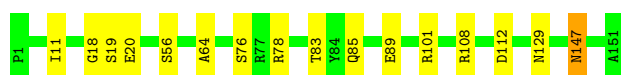
- Molecule 39: 30S ribosomal protein S6

Chain f:  87% 9%



- Molecule 40: 30S ribosomal protein S7

Chain g:  89% 10%



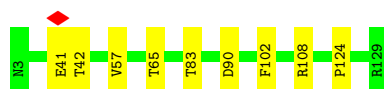
- Molecule 41: 30S ribosomal protein S8

Chain h:  88% 12%



- Molecule 42: 30S ribosomal protein S9

Chain i:  93% 7%

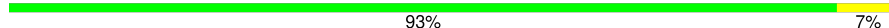


- Molecule 43: 30S ribosomal protein S10

Chain j:  91% 8%



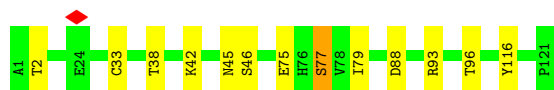
- Molecule 44: 30S ribosomal protein S11

Chain k:  93% 7%



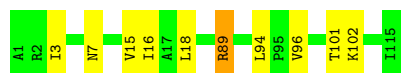
- Molecule 45: 30S ribosomal protein S12

Chain l:  89% 10%



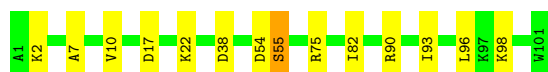
- Molecule 46: 30S ribosomal protein S13

Chain m:  91% 8%



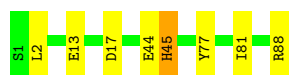
- Molecule 47: 30S ribosomal protein S14

Chain n:  86% 13%



- Molecule 48: 30S ribosomal protein S15

Chain o:  91% 8%



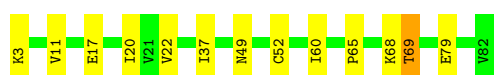
- Molecule 49: 30S ribosomal protein S16

Chain p:  87% 13%



- Molecule 50: 30S ribosomal protein S17

Chain q:  84% 15%



- Molecule 51: 30S ribosomal protein S18

Chain r:  80% 18%



- Molecule 52: 30S ribosomal protein S19

Chain s:  91% 9%



- Molecule 53: 30S ribosomal protein S20

Chain t:  91% 9%



- Molecule 54: 30S ribosomal protein S21

Chain u:  77% 18% 5%



- Molecule 55: tRNA-fMet

Chain v:  65% 31%



- Molecule 55: tRNA-fMet

Chain w:  8% 55% 31% 13%



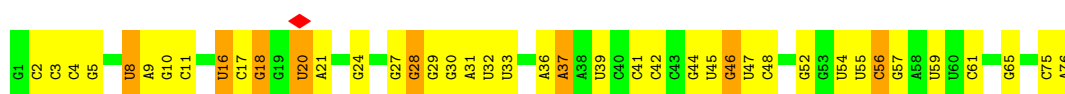
- Molecule 56: mRNA

Chain x:  67% 25% 8%

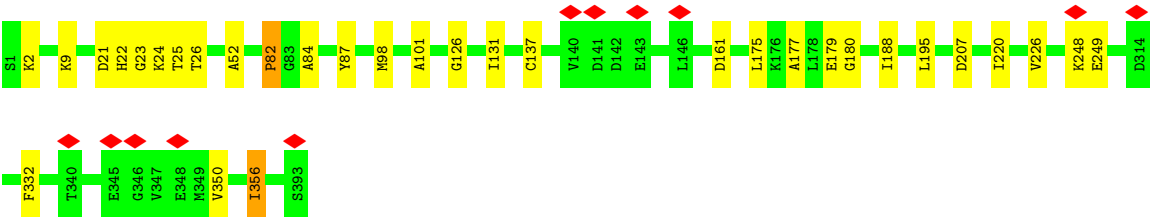
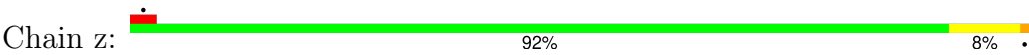


- Molecule 57: Phe-tRNA-Phe

Chain y:  46% 43% 11%



- Molecule 58: Elongation factor Tu 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58475	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.288	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.00532	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, 5MU, 7MG, 4SU, MG, K, 2MA, 3TD, 6MZ, GTP, OMU, OMC, FME, OMG, 4OC, UR3, 2MG, 1MG, PSU, MIA, MA6, 5MC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/69174	0.76	48/107907 (0.0%)
2	B	0.39	0/2876	0.77	0/4483
3	C	0.50	0/2121	0.78	0/2852
4	D	0.49	0/1578	0.77	2/2124 (0.1%)
5	E	0.49	0/1563	0.82	0/2103
6	F	0.55	0/1434	0.82	0/1926
7	G	0.53	0/1324	0.74	0/1794
8	H	0.62	0/1122	0.81	0/1515
9	I	0.69	0/1046	0.92	0/1410
10	J	0.49	0/1143	0.80	0/1540
11	K	0.50	0/947	0.76	0/1268
12	L	0.51	0/1052	0.88	0/1401
13	M	0.49	0/1093	0.79	0/1460
14	N	0.53	0/964	0.86	0/1289
15	O	0.52	0/902	0.84	0/1209
16	P	0.48	0/929	0.75	0/1242
17	Q	0.49	0/946	0.88	0/1260
18	R	0.48	0/823	0.70	0/1100
19	S	0.49	0/852	0.83	0/1142
20	T	0.50	0/736	0.76	0/984
21	U	0.47	0/787	0.73	0/1051
22	V	0.49	0/752	0.74	0/1008
23	W	0.47	0/579	0.68	0/767
24	X	0.48	0/635	0.72	0/848
25	Y	0.53	0/495	0.87	0/658
26	Z	0.52	0/438	0.78	0/586
27	0	0.45	0/440	0.81	0/588
28	1	0.49	0/424	0.69	0/565
29	2	0.52	0/370	0.97	0/487
30	3	0.46	0/513	0.84	0/676
31	4	0.46	0/303	0.75	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.67	0/1001	0.84	0/1350
33	6	0.57	0/531	0.79	0/709
34	a	0.39	0/36725	0.76	25/57285 (0.0%)
35	b	0.55	0/1735	0.79	0/2338
36	c	0.53	0/1651	0.80	0/2225
37	d	0.60	0/1665	0.82	0/2227
38	e	0.52	0/1180	0.84	0/1587
39	f	0.56	0/835	0.81	2/1128 (0.2%)
40	g	0.53	0/1195	0.82	0/1602
41	h	0.52	0/989	0.80	0/1326
42	i	0.56	0/1034	0.76	0/1375
43	j	0.55	0/796	0.74	0/1077
44	k	0.54	0/885	0.78	0/1195
45	l	0.56	0/954	0.78	0/1282
46	m	0.56	0/900	0.84	0/1204
47	n	0.53	0/822	0.79	0/1095
48	o	0.50	0/722	0.83	0/964
49	p	0.56	0/659	0.78	0/884
50	q	0.56	0/657	0.76	0/881
51	r	0.60	0/544	0.80	0/731
52	s	0.55	0/652	0.75	0/877
53	t	0.54	0/671	0.88	0/888
54	u	0.64	0/550	0.92	0/728
55	v	0.41	1/1747 (0.1%)	0.74	0/2721
55	w	0.40	0/1747	0.98	5/2721 (0.2%)
56	x	0.37	0/280	0.77	0/433
57	y	0.40	0/1607	0.73	1/2501 (0.0%)
58	z	0.57	0/3086	0.78	0/4175
All	All	0.43	1/164181 (0.0%)	0.77	83/245149 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
34	a	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	7	4SU	O3'-P	5.46	1.61	1.56

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	117	U	O3'-P-O5'	23.50	139.25	104.00
55	w	117	U	P-O3'-C3'	22.09	153.34	120.20
34	a	1399	C	C2'-C3'-O3'	10.11	124.67	109.50
34	a	1305	G	C2'-C3'-O3'	9.84	124.27	109.50
1	A	301	G	C4'-C3'-O3'	9.44	123.55	109.40
1	A	242	G	C2'-C3'-O3'	9.35	123.52	109.50
1	A	1022	G	C2'-C3'-O3'	9.15	123.23	109.50
1	A	204	A	C4'-C3'-O3'	9.15	123.12	109.40
1	A	2407	A	C2'-C3'-O3'	8.83	126.94	113.70
1	A	1475	G	C2'-C3'-O3'	8.43	122.15	109.50
1	A	1484	U	N1-C1'-C2'	8.41	124.61	112.00
1	A	614	A	C4'-C3'-O3'	-8.34	96.89	109.40
34	a	1432	G	C2'-C3'-O3'	8.32	121.99	109.50
1	A	859	G	C4'-C3'-O3'	8.31	121.87	109.40
34	a	246	A	C4'-C3'-O3'	8.03	121.44	109.40
55	w	117	U	OP1-P-O3'	-7.89	84.33	108.00
1	A	1730	U	C2'-C3'-O3'	7.89	121.33	109.50
34	a	1201	A	C2'-C3'-O3'	7.58	120.86	109.50
34	a	1190	G	C2'-C3'-O3'	7.56	120.83	109.50
1	A	2296	U	C4'-C3'-O3'	7.55	120.72	109.40
1	A	265	A	C4'-C3'-O3'	7.51	120.66	109.40
34	a	574	A	C4'-C3'-O3'	-7.49	101.76	113.00
1	A	2391	G	C4'-C3'-O3'	7.45	124.17	113.00
34	a	495	A	C4'-C3'-O3'	7.44	120.56	109.40
1	A	1070	A	C2'-C3'-O3'	7.04	120.06	109.50
55	w	75	C	C4'-C3'-O3'	6.96	119.83	109.40
1	A	613	A	C2'-C3'-O3'	-6.79	99.32	109.50
1	A	1051	G	N9-C1'-C2'	6.78	122.17	112.00
1	A	360	U	C4'-C3'-O3'	6.58	119.27	109.40
34	a	280	C	C4'-C3'-O3'	6.51	119.17	109.40
1	A	2566	A	C4'-C3'-O3'	6.46	119.08	109.40
1	A	2475	C	N1-C1'-C2'	6.27	121.40	112.00
34	a	960	U	C4'-C3'-O3'	6.22	118.73	109.40
1	A	51	G	C4'-C3'-O3'	6.15	118.63	109.40
1	A	1940	U	C2'-C3'-O3'	6.11	118.67	109.50
1	A	1113	U	C2'-C3'-O3'	-5.96	104.76	113.70
34	a	1448	C	N1-C1'-C2'	5.95	120.92	112.00
1	A	1694	C	C4'-C3'-O3'	5.94	118.31	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	960	U	C2'-C3'-O3'	5.84	118.26	109.50
34	a	1297	G	C2'-C3'-O3'	5.82	118.23	109.50
34	a	85	U	C2'-C3'-O3'	-5.80	105.00	113.70
34	a	214	C	C4'-C3'-O3'	-5.77	104.35	113.00
1	A	2712	C	C2'-C3'-O3'	5.73	118.10	109.50
1	A	1106	G	C1'-C2'-O2'	5.72	120.38	111.80
1	A	1254	A	C4'-C3'-O3'	-5.71	104.43	113.00
1	A	1945	G	C4'-C3'-O3'	-5.71	104.43	113.00
34	a	94	G	C2'-C3'-O3'	5.64	117.96	109.50
1	A	1050	A	C2'-C3'-O3'	5.62	122.14	113.70
1	A	1020	A	C4'-C3'-O3'	5.61	117.81	109.40
1	A	2712	C	C4'-C3'-O3'	5.58	117.78	109.40
34	a	1084	G	C4'-C3'-O3'	-5.58	104.62	113.00
1	A	1536	C	C2'-C3'-O3'	5.57	122.06	113.70
34	a	1272	G	C4'-C3'-O3'	-5.56	104.67	113.00
1	A	1050	A	O4'-C1'-C2'	-5.53	102.07	107.60
1	A	710	U	C2'-C3'-O3'	5.49	121.93	113.70
1	A	2474	U	N1-C1'-C2'	5.40	120.10	112.00
1	A	2467	C	C4'-C3'-O3'	-5.36	104.96	113.00
34	a	382	A	C4'-C3'-O3'	5.35	121.03	113.00
4	D	151	THR	CA-C-N	-5.33	113.42	118.97
4	D	151	THR	C-N-CA	-5.33	113.42	118.97
1	A	2472	G	N9-C1'-C2'	5.33	119.99	112.00
34	a	384	G	N9-C1'-C2'	5.32	121.98	114.00
1	A	1069	A	C2'-C3'-O3'	-5.28	105.79	113.70
34	a	63	C	C3'-C2'-O2'	5.27	118.61	110.70
1	A	12	U	N1-C1'-C2'	5.25	119.88	112.00
1	A	84	A	C4'-C3'-O3'	5.25	117.27	109.40
1	A	1507	C	C3'-C2'-O2'	5.24	118.56	110.70
34	a	429	U	C4'-C3'-O3'	5.20	117.20	109.40
34	a	379	C	C4'-C3'-O3'	-5.19	105.21	113.00
34	a	635	A	C4'-C3'-O3'	-5.18	105.22	113.00
1	A	1481	U	C2'-C3'-O3'	5.14	121.42	113.70
1	A	941	A	C4'-C3'-O3'	-5.14	105.29	113.00
39	f	17	GLN	CA-C-N	5.13	123.47	120.24
39	f	17	GLN	C-N-CA	5.13	123.47	120.24
1	A	982	C	C2'-C3'-O3'	-5.12	106.01	113.70
1	A	543	G	C2'-C3'-O3'	-5.12	106.02	113.70
34	a	712	A	C4'-C3'-O3'	-5.12	105.33	113.00
1	A	2528	U	C3'-C2'-O2'	5.11	118.37	110.70
1	A	1940	U	C4'-C3'-O3'	5.08	117.01	109.40
57	y	2	C	C2'-C3'-O3'	5.06	121.29	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	783	A	C4'-C3'-O3'	5.04	120.56	113.00
55	w	69	C	C2'-C3'-O3'	5.01	121.22	113.70
1	A	2326	C	C3'-C2'-O2'	5.01	118.21	110.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1054	A	Sidechain
34	a	141	G	Sidechain
34	a	222	C	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62277	0	31337	505	0
2	B	2572	0	1302	19	0
3	C	2082	0	2157	12	0
4	D	1557	0	1604	5	0
5	E	1544	0	1607	5	0
6	F	1410	0	1447	7	0
7	G	1304	0	1348	3	0
8	H	1111	0	1148	2	0
9	I	1032	0	1088	8	0
10	J	1120	0	1151	7	0
11	K	938	0	1012	3	0
12	L	1043	0	1123	7	0
13	M	1074	0	1157	5	0
14	N	951	0	994	4	0
15	O	892	0	923	4	0
16	P	917	0	965	6	0
17	Q	933	0	1006	7	0
18	R	810	0	834	6	0
19	S	845	0	909	4	0
20	T	730	0	795	2	0
21	U	779	0	834	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	739	0	763	3	0
23	W	572	0	593	2	0
24	X	625	0	655	0	0
25	Y	494	0	530	1	0
26	Z	434	0	477	2	0
27	0	434	0	448	5	0
28	1	417	0	451	0	0
29	2	367	0	405	6	0
30	3	504	0	574	0	0
31	4	302	0	343	5	0
32	5	988	0	1025	3	0
33	6	522	0	524	1	0
34	a	33050	0	16652	300	0
35	b	1704	0	1732	3	0
36	c	1624	0	1699	8	0
37	d	1643	0	1710	5	0
38	e	1164	0	1212	11	0
39	f	817	0	808	15	0
40	g	1181	0	1240	5	0
41	h	979	0	1034	9	0
42	i	1022	0	1070	1	0
43	j	786	0	828	3	0
44	k	869	0	878	0	0
45	l	940	0	1001	3	0
46	m	891	0	955	5	0
47	n	810	0	852	5	0
48	o	714	0	737	2	0
49	p	649	0	666	5	0
50	q	648	0	691	4	0
51	r	535	0	552	4	0
52	s	637	0	665	3	0
53	t	665	0	714	1	0
54	u	544	0	579	4	0
55	v	1644	0	840	1	0
55	w	1644	0	840	14	0
56	x	252	0	130	1	0
57	y	1632	0	843	8	0
58	z	3031	0	3052	19	0
59	A	10	0	10	0	0
60	0	3	0	0	0	0
60	2	1	0	0	0	0
60	A	1011	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	B	37	0	0	0	0
60	C	1	0	0	0	0
60	D	2	0	0	0	0
60	E	1	0	0	0	0
60	M	2	0	0	0	0
60	N	1	0	0	0	0
60	Q	1	0	0	0	0
60	T	1	0	0	0	0
60	W	1	0	0	0	0
60	a	392	0	0	0	0
60	d	1	0	0	0	0
60	e	1	0	0	0	0
60	i	1	0	0	0	0
60	u	1	0	0	0	0
60	v	6	0	0	0	0
60	w	2	0	0	0	0
60	x	1	0	0	0	0
60	y	2	0	0	0	0
60	z	2	0	0	0	0
61	A	6	0	0	0	0
61	a	1	0	0	0	0
62	z	11	0	8	0	0
63	z	32	0	12	16	0
64	0	2	0	0	0	0
64	1	1	0	0	0	0
64	2	2	0	0	0	0
64	3	1	0	0	0	0
64	A	828	0	0	0	0
64	B	29	0	0	0	0
64	C	5	0	0	0	0
64	D	6	0	0	0	0
64	E	5	0	0	0	0
64	J	4	0	0	0	0
64	L	5	0	0	0	0
64	N	1	0	0	0	0
64	O	1	0	0	0	0
64	Q	3	0	0	0	0
64	R	1	0	0	0	0
64	S	3	0	0	0	0
64	W	2	0	0	0	0
64	X	3	0	0	0	0
64	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	a	253	0	0	1	0
64	c	1	0	0	0	0
64	i	1	0	0	0	0
64	j	1	0	0	0	0
64	l	2	0	0	0	0
64	m	1	0	0	0	0
64	o	1	0	0	0	0
64	q	1	0	0	0	0
64	s	3	0	0	0	0
64	u	1	0	0	0	0
64	v	3	0	0	0	0
64	w	1	0	0	0	0
64	x	1	0	0	0	0
64	y	2	0	0	0	0
All	All	155100	0	103539	1030	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1030) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:182:A:N1	34:a:185:U:O4	1.63	1.31
1:A:1105:U:N3	1:A:1106:G:N9	1.79	1.28
1:A:1021:A:N1	1:A:1141:U:O4	1.70	1.24
1:A:1054:A:N6	1:A:1106:G:N7	1.91	1.18
1:A:1915:3TD:C1'	1:A:1915:3TD:O4'	1.66	1.18
1:A:1054:A:N6	1:A:1106:G:C8	2.10	1.18
34:a:827:U:O4	34:a:872:A:N1	1.79	1.15
34:a:141:G:O6	34:a:222:C:C2	1.99	1.14
39:f:38:ARG:HG3	39:f:63:ASN:HB3	1.32	1.12
34:a:141:G:C6	34:a:222:C:O2	2.01	1.12
1:A:2013:A:N1	1:A:2613:U:O4	1.83	1.11
63:z:402:GTP:H8	63:z:402:GTP:H5''	1.07	1.08
1:A:1042:G:O6	1:A:1113:U:O2	1.74	1.06
34:a:141:G:C6	34:a:222:C:C2	2.43	1.05
1:A:1105:U:C4	1:A:1106:G:N9	2.09	1.05
58:z:25:THR:OG1	63:z:402:GTP:O1B	1.73	1.05
1:A:1050:A:C8	1:A:1051:G:C8	2.45	1.04
39:f:38:ARG:CG	39:f:63:ASN:HB3	1.86	1.04
55:w:17:C:C5	55:w:117:U:H5	1.77	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:w:18:G:O2'	55:w:19:G:OP1	1.74	1.02
1:A:286:U:O2	1:A:354:A:N6	1.93	1.00
55:w:17:C:C5	55:w:117:U:C5	2.49	1.00
34:a:142:G:N2	34:a:222:C:O4'	1.94	1.00
2:B:4:C:N4	2:B:116:G:O6	1.95	1.00
1:A:1105:U:N3	1:A:1106:G:C1'	2.25	0.99
1:A:1050:A:N6	1:A:2751:G:C6	2.29	0.99
34:a:69:G:N2	34:a:100:G:O6	1.96	0.98
34:a:500:G:O6	34:a:545:C:N3	1.97	0.97
63:z:402:GTP:H5''	63:z:402:GTP:C8	2.00	0.97
34:a:936:C:N3	34:a:1379:G:O6	1.97	0.97
1:A:1472:C:N3	1:A:1519:G:O6	1.98	0.96
1:A:1050:A:C6	1:A:2751:G:C6	2.54	0.95
1:A:1050:A:N6	1:A:2751:G:O6	2.02	0.93
1:A:1105:U:N3	1:A:1106:G:C4	2.24	0.93
1:A:1052:C:O2	1:A:1107:G:N1	2.01	0.93
55:w:17:C:H5	55:w:117:U:C5	1.87	0.92
1:A:843:G:O6	1:A:935:C:N3	2.02	0.92
34:a:605:U:O2	34:a:633:G:N1	2.05	0.89
1:A:713:G:N2	1:A:718:A:N7	2.19	0.89
34:a:153:C:N4	34:a:168:G:O6	2.05	0.89
58:z:23:GLY:HA2	63:z:402:GTP:O1A	1.71	0.88
1:A:1054:A:N6	1:A:1106:G:C5	2.31	0.88
1:A:2471:A:H2'	1:A:2472:G:O4'	1.73	0.88
1:A:1054:A:N1	1:A:1106:G:C2'	2.37	0.88
46:m:15:VAL:HG23	46:m:16:ILE:HD12	1.56	0.87
1:A:708:G:O6	1:A:722:A:N6	2.07	0.86
2:B:39:A:O2'	2:B:46:A:N1	2.09	0.86
58:z:23:GLY:CA	63:z:402:GTP:O1A	2.24	0.86
1:A:272:A:N1	1:A:365:U:O4	2.09	0.85
55:w:117:U:O2'	55:w:18:G:OP1	1.95	0.85
1:A:2030:6MZ:O2'	1:A:2031:A:P	2.34	0.85
1:A:283:G:O6	1:A:357:C:H1'	1.77	0.84
58:z:24:LYS:NZ	63:z:402:GTP:O1G	2.08	0.84
1:A:1050:A:H8	1:A:1051:G:C8	1.91	0.84
34:a:417:G:H2'	34:a:418:C:H5'	1.59	0.84
34:a:1397:C:OP2	56:x:23:C:N4	2.10	0.83
34:a:936:C:O2	34:a:1379:G:N1	2.09	0.83
1:A:1047:G:H2'	1:A:1110:G:N2	1.94	0.83
34:a:601:G:H2'	34:a:602:A:H5'	1.60	0.83
34:a:42:G:N3	34:a:622:A:C2	2.47	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:U:C2	1:A:1106:G:O4'	2.32	0.83
1:A:288:U:O4	1:A:352:A:C6	2.32	0.83
58:z:21:ASP:HA	63:z:402:GTP:O2A	1.77	0.82
1:A:1484:U:H2'	1:A:1485:U:C6	2.14	0.82
34:a:263:A:O2'	34:a:264:C:O2	1.98	0.81
1:A:2474:U:H3'	1:A:2475:C:C5	2.16	0.81
1:A:2320:U:H4'	1:A:2321:U:H5''	1.63	0.81
1:A:2297:A:N1	1:A:2321:U:C4	2.49	0.80
1:A:1021:A:N6	1:A:1141:U:H3	1.80	0.80
1:A:1050:A:C8	1:A:1051:G:H8	1.96	0.80
1:A:278:A:N6	1:A:362:A:O4'	2.15	0.80
34:a:137:U:O2	34:a:226:G:N1	2.15	0.79
1:A:1052:C:N3	1:A:1107:G:O6	2.16	0.79
34:a:137:U:N3	34:a:226:G:O6	2.15	0.79
34:a:141:G:N7	34:a:223:A:C2	2.51	0.79
55:w:18:G:O2'	55:w:19:G:P	2.41	0.78
1:A:1021:A:H61	1:A:1141:U:H3	1.28	0.78
1:A:1485:U:H2'	1:A:1486:U:C6	2.18	0.78
1:A:2840:C:H5''	14:N:53:THR:HG21	1.65	0.77
34:a:401:C:O2'	34:a:621:A:N3	2.18	0.77
1:A:1105:U:C2	1:A:1106:G:C1'	2.67	0.77
1:A:1779:U:C5	1:A:1784:A:N7	2.54	0.76
16:P:59:THR:HG22	16:P:72:VAL:HG22	1.68	0.75
1:A:1054:A:C2	1:A:1106:G:O2'	2.39	0.74
34:a:618:C:C2	34:a:622:A:N6	2.56	0.74
1:A:709:U:C4	1:A:722:A:N1	2.55	0.74
1:A:2292:U:H2'	1:A:2293:G:H5'	1.70	0.74
34:a:404:G:C2	34:a:498:A:N3	2.56	0.74
34:a:42:G:N3	34:a:622:A:N3	2.36	0.73
34:a:605:U:O2	34:a:633:G:C6	2.41	0.73
34:a:632:U:H5''	34:a:633:G:H5''	1.70	0.73
34:a:827:U:H3	34:a:872:A:N6	1.87	0.73
1:A:2028:U:H2'	1:A:2029:G:C8	2.24	0.73
1:A:2472:G:H1	1:A:2475:C:H2'	1.54	0.73
34:a:546:A:HO2'	34:a:548:G:HO2'	1.36	0.73
1:A:80:G:H2'	1:A:81:G:H5'	1.71	0.73
34:a:618:C:O2	34:a:622:A:N6	2.21	0.73
52:s:48:ILE:HD11	52:s:70:LEU:HD22	1.70	0.73
1:A:1054:A:C4	1:A:1106:G:C2	2.77	0.72
1:A:568:U:H1'	1:A:2030:6MZ:H9C1	1.72	0.71
34:a:74:A:C2	34:a:97:G:N2	2.58	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:202:G:O6	34:a:215:C:N3	2.22	0.71
1:A:2028:U:C4	1:A:2029:G:C6	2.78	0.71
34:a:546:A:O2'	34:a:548:G:O2'	2.09	0.71
1:A:1064:C:N4	1:A:1069:A:OP2	2.23	0.71
1:A:2320:U:H4'	1:A:2321:U:C5'	2.20	0.71
1:A:1483:G:N2	1:A:1484:U:C2	2.59	0.70
1:A:1051:G:O6	1:A:1109:C:C2	2.44	0.70
1:A:1105:U:H3	1:A:1106:G:C1'	1.97	0.70
1:A:1507:C:C4	1:A:1508:A:N6	2.60	0.70
1:A:273:G:C8	1:A:365:U:C4	2.80	0.70
58:z:23:GLY:N	63:z:402:GTP:O1A	2.25	0.70
1:A:2297:A:C6	1:A:2321:U:O4	2.46	0.69
1:A:2720:U:OP1	16:P:52:ARG:NH2	2.26	0.69
34:a:182:A:N3	34:a:184:G:C6	2.61	0.69
1:A:286:U:C2	1:A:354:A:N6	2.60	0.69
1:A:709:U:O4	1:A:722:A:N1	2.25	0.69
1:A:278:A:C6	1:A:361:G:H8	2.11	0.69
39:f:38:ARG:HD2	39:f:63:ASN:ND2	2.08	0.69
34:a:404:G:N3	34:a:498:A:H2	1.91	0.68
39:f:38:ARG:HG3	39:f:63:ASN:CB	2.19	0.68
1:A:288:U:O4	1:A:352:A:N6	2.27	0.68
1:A:1050:A:C6	1:A:2751:G:C5	2.82	0.68
34:a:417:G:C2'	34:a:418:C:H5'	2.22	0.68
34:a:193:C:H2'	34:a:194:C:C6	2.29	0.67
55:w:17:C:C6	55:w:117:U:H5	2.11	0.67
1:A:283:G:C8	1:A:358:U:C4	2.83	0.67
34:a:848:C:H6	34:a:848:C:O5'	1.78	0.67
34:a:454:G:O6	34:a:478:A:N1	2.27	0.67
1:A:1021:A:C2	1:A:1141:U:O4	2.46	0.67
1:A:2298:A:C4	1:A:2321:U:C5	2.83	0.67
34:a:380:G:C2	34:a:384:G:O6	2.48	0.67
1:A:1537:G:N1	1:A:1538:G:N3	2.43	0.66
1:A:2297:A:N1	1:A:2321:U:O4	2.28	0.66
34:a:601:G:C2'	34:a:602:A:H5'	2.24	0.66
1:A:278:A:C2	1:A:279:A:N7	2.64	0.66
1:A:924:G:H2'	1:A:925:A:H5'	1.77	0.66
1:A:2856:A:H2'	1:A:2857:G:H5'	1.76	0.66
1:A:288:U:C4	1:A:352:A:N1	2.63	0.66
1:A:2292:U:C2'	1:A:2293:G:H5'	2.25	0.66
1:A:2030:6MZ:O2'	1:A:2031:A:OP2	2.13	0.66
1:A:2471:A:C2	1:A:2479:U:N3	2.63	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:A:C2	1:A:359:G:C2	2.84	0.66
5:E:46:GLN:HB3	5:E:83:VAL:HG11	1.78	0.65
1:A:272:A:N1	1:A:365:U:C4	2.64	0.65
1:A:276:U:H2'	1:A:361:G:O6	1.96	0.65
34:a:31:G:C2	34:a:306:A:O2'	2.49	0.65
34:a:382:A:C5	34:a:383:A:C2	2.85	0.65
34:a:446:G:O6	34:a:488:C:N3	2.29	0.65
34:a:131:A:N1	34:a:230:G:O6	2.29	0.65
1:A:710:U:C2	1:A:711:G:C8	2.84	0.65
1:A:1105:U:C5	1:A:1106:G:C8	2.58	0.65
1:A:219:A:N3	1:A:234:U:O2'	2.30	0.64
1:A:278:A:N7	1:A:362:A:N3	2.44	0.64
1:A:362:A:N7	1:A:363:G:C6	2.64	0.64
1:A:2030:6MZ:OP2	1:A:2031:A:H8	1.80	0.64
34:a:922:G:O2'	34:a:1398:A:N1	2.29	0.64
34:a:64:G:N2	34:a:69:G:N7	2.46	0.64
41:h:10:LEU:HD22	41:h:74:ILE:HD11	1.79	0.64
1:A:221:A:N7	1:A:427:U:H5	1.96	0.64
1:A:1607:C:N4	1:A:1622:G:OP2	2.29	0.64
34:a:454:G:C6	34:a:478:A:N1	2.66	0.64
1:A:543:G:H3'	1:A:544:C:H5''	1.80	0.64
1:A:1050:A:N7	1:A:1051:G:N7	2.46	0.64
39:f:38:ARG:CG	39:f:63:ASN:CB	2.70	0.63
3:C:121:ALA:HB3	3:C:129:LEU:HD21	1.80	0.63
1:A:1068:G:H1	1:A:1095:A:H2'	1.64	0.63
1:A:1109:C:H41	1:A:1110:G:H21	1.46	0.63
1:A:550:C:N4	1:A:551:G:C6	2.67	0.63
1:A:1739:A:H2'	1:A:1740:G:O4'	1.99	0.63
34:a:182:A:N1	34:a:185:U:C4	2.59	0.63
1:A:1297:C:OP1	1:A:2710:C:H4'	1.99	0.62
7:G:32:LEU:HB3	7:G:74:MET:HE3	1.81	0.62
1:A:272:A:C2	1:A:366:C:C2	2.87	0.62
1:A:2020:A:N7	27:0:5:ASN:ND2	2.46	0.62
38:e:106:ALA:HB2	38:e:124:ALA:HB3	1.80	0.62
1:A:2472:G:N1	1:A:2475:C:H2'	2.14	0.62
1:A:363:G:H2'	1:A:364:C:O4'	1.99	0.62
1:A:2030:6MZ:OP2	1:A:2030:6MZ:H4'	1.98	0.62
34:a:404:G:C2	34:a:498:A:C2	2.87	0.62
34:a:632:U:C5'	34:a:633:G:H5''	2.30	0.62
1:A:2030:6MZ:HA	1:A:2031:A:P	2.23	0.62
1:A:290:U:O2'	1:A:291:G:O5'	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:137:U:C2	34:a:226:G:O6	2.52	0.62
1:A:517:C:OP1	27:0:12:ARG:NH2	2.32	0.62
1:A:1054:A:N3	1:A:1106:G:C2	2.68	0.62
1:A:900:A:C2	1:A:901:C:O4'	2.53	0.61
39:f:38:ARG:CD	39:f:63:ASN:CB	2.77	0.61
55:w:17:C:H5	55:w:117:U:C4	2.18	0.61
1:A:278:A:N1	1:A:279:A:N7	2.48	0.61
34:a:456:A:C2	34:a:477:C:C2	2.88	0.61
34:a:203:G:N2	34:a:204:G:O6	2.32	0.61
34:a:377:G:N1	34:a:387:U:O2	2.34	0.61
1:A:1021:A:N1	1:A:1141:U:C4	2.63	0.61
1:A:2627:G:O2'	1:A:2781:A:N1	2.30	0.61
1:A:1328:A:H2'	1:A:1330:C:C5	2.36	0.61
1:A:900:A:H2'	1:A:900:A:N3	2.15	0.61
3:C:79:ARG:NH1	3:C:81:GLU:OE2	2.34	0.61
34:a:132:C:N3	34:a:230:G:O6	2.33	0.60
1:A:287:G:C6	1:A:288:U:C5	2.89	0.60
1:A:1005:C:O2'	10:J:30:THR:HG21	2.02	0.60
34:a:827:U:C4	34:a:872:A:N1	2.67	0.60
1:A:133:U:H2'	1:A:134:G:O4'	2.02	0.60
1:A:1936:A:H2	1:A:1943:U:H3	1.49	0.60
34:a:2:A:N3	34:a:613:C:O2'	2.27	0.60
34:a:141:G:O2'	34:a:142:G:O4'	2.19	0.60
1:A:585:G:N7	17:Q:5:ARG:NH1	2.49	0.60
34:a:827:U:N3	34:a:872:A:N6	2.45	0.60
34:a:1240:U:O4	40:g:108:ARG:NH1	2.35	0.60
1:A:288:U:O4	1:A:352:A:N1	2.35	0.60
1:A:1539:U:H2'	1:A:1540:G:C8	2.36	0.60
1:A:2328:A:H2'	1:A:2329:U:C6	2.37	0.60
1:A:1140:C:O2	1:A:1140:C:O5'	2.20	0.60
1:A:1538:G:H2'	1:A:1539:U:O4'	2.02	0.60
1:A:1867:G:O6	1:A:1874:C:C4	2.55	0.60
34:a:141:G:N3	34:a:141:G:H2'	2.17	0.60
1:A:1721:G:O2'	1:A:1739:A:N6	2.35	0.59
34:a:264:C:O2	34:a:264:C:O4'	2.20	0.59
57:y:29:G:N2	57:y:41:C:N3	2.50	0.59
34:a:473:U:C2	34:a:474:G:C8	2.90	0.59
1:A:314:C:H2'	1:A:315:G:H5'	1.85	0.59
34:a:512:U:H2'	34:a:513:C:C5'	2.32	0.59
34:a:839:C:N3	34:a:847:G:O6	2.34	0.59
1:A:1054:A:H2'	1:A:1106:G:N2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:102:LEU:HD21	6:F:129:MET:HE1	1.84	0.59
34:a:605:U:C2	34:a:633:G:O6	2.56	0.59
1:A:900:A:C2	1:A:901:C:C1'	2.85	0.59
1:A:1779:U:H5	1:A:1784:A:N7	2.01	0.59
57:y:18:G:O2'	57:y:57:G:N2	2.36	0.59
2:B:105:G:H2'	2:B:106:G:H5'	1.84	0.59
29:2:12:ARG:HE	29:2:44:VAL:HG21	1.68	0.59
1:A:639:U:H2'	1:A:640:C:C6	2.38	0.59
1:A:1054:A:C5	1:A:1106:G:C6	2.90	0.59
34:a:708:C:H2'	34:a:709:U:H5'	1.84	0.59
1:A:710:U:H2'	1:A:711:G:H5''	1.84	0.59
34:a:160:A:H1'	34:a:344:A:N7	2.18	0.58
1:A:2029:G:O5'	1:A:2029:G:H8	1.85	0.58
1:A:283:G:O6	1:A:357:C:O2	2.22	0.58
34:a:455:G:N2	34:a:477:C:N3	2.50	0.58
1:A:80:G:C2'	1:A:81:G:H5'	2.34	0.58
6:F:10:GLU:O	6:F:12:VAL:N	2.36	0.58
34:a:827:U:H3	34:a:872:A:H61	1.43	0.58
1:A:2101:A:N6	1:A:2188:U:C4	2.72	0.58
34:a:73:C:H2'	34:a:74:A:C8	2.39	0.58
1:A:1039:A:N1	1:A:1116:G:O6	2.36	0.58
1:A:528:A:C2	1:A:2043:C:H4'	2.39	0.58
1:A:2472:G:O6	1:A:2475:C:H3'	2.04	0.58
1:A:2474:U:H3'	1:A:2475:C:H5	1.68	0.58
34:a:404:G:N3	34:a:498:A:C2	2.71	0.58
52:s:10:ILE:HD12	52:s:40:PHE:CD2	2.38	0.58
1:A:1617:C:P	1:A:1617:C:H3'	2.44	0.58
1:A:1754:A:N1	1:A:2716:C:O2'	2.34	0.58
36:c:63:ILE:HD13	36:c:94:ALA:HB1	1.85	0.58
43:j:57:VAL:HG12	43:j:58:ASN:H	1.68	0.58
1:A:709:U:H2'	1:A:710:U:O4'	2.03	0.57
34:a:69:G:C2	34:a:100:G:O6	2.56	0.57
54:u:9:GLU:HB2	54:u:10:PRO:CD	2.34	0.57
1:A:138:U:O2	1:A:138:U:H2'	2.03	0.57
1:A:1024:G:H1	1:A:1140:C:H5	1.52	0.57
1:A:2472:G:O2'	1:A:2529:G:N2	2.37	0.57
1:A:1140:C:O2	1:A:1140:C:O4'	2.22	0.57
34:a:633:G:H2'	34:a:634:C:C6	2.39	0.57
1:A:272:A:C6	1:A:365:U:O4	2.56	0.57
1:A:713:G:N2	1:A:719:C:C2	2.72	0.57
1:A:1036:G:O6	1:A:1119:U:C2	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:155:A:C2	34:a:167:A:C6	2.92	0.57
34:a:512:U:H2'	34:a:513:C:H5'	1.87	0.57
34:a:137:U:O2	34:a:226:G:C6	2.57	0.57
63:z:402:GTP:H8	63:z:402:GTP:C5'	1.99	0.57
1:A:287:G:N7	1:A:354:A:C6	2.73	0.57
1:A:1109:C:N4	1:A:1110:G:H21	2.03	0.57
1:A:900:A:H2	1:A:901:C:O4'	1.86	0.57
1:A:2013:A:N1	1:A:2613:U:C4	2.68	0.57
34:a:179:A:H2'	34:a:180:U:O4'	2.04	0.57
34:a:382:A:C8	34:a:383:A:C2	2.93	0.57
1:A:321:U:C2	5:E:159:LEU:HD21	2.40	0.57
1:A:710:U:N3	1:A:711:G:N7	2.52	0.57
1:A:1021:A:H3'	1:A:1022:G:H5''	1.85	0.57
1:A:1170:C:H2'	1:A:1171:G:C8	2.40	0.57
34:a:69:G:N2	34:a:71:A:C6	2.73	0.57
34:a:417:G:O6	34:a:426:U:O2	2.22	0.57
39:f:29:ILE:HG21	39:f:64:VAL:HG21	1.86	0.57
58:z:82:PRO:O	63:z:402:GTP:O3G	2.23	0.56
1:A:1482:G:H2'	1:A:1483:G:H5'	1.87	0.56
3:C:69:ASN:O	3:C:70:LYS:C	2.47	0.56
34:a:382:A:C4	34:a:383:A:C2	2.93	0.56
1:A:1483:G:N3	1:A:1484:U:C6	2.73	0.56
34:a:602:A:N1	34:a:636:U:C2	2.74	0.56
40:g:85:GLN:HB2	40:g:147:ASN:HD22	1.71	0.56
1:A:553:G:H2'	1:A:554:U:O4'	2.05	0.56
1:A:2698:U:H2'	1:A:2699:C:C6	2.41	0.56
34:a:936:C:N3	34:a:1379:G:C6	2.73	0.56
58:z:220:ILE:HD12	58:z:226:VAL:HG21	1.87	0.56
1:A:1483:G:O2'	1:A:1484:U:H6	1.89	0.56
9:I:27:LEU:HD21	9:I:37:PHE:CG	2.40	0.56
1:A:2297:A:C2	1:A:2321:U:C5	2.94	0.56
1:A:1054:A:C8	1:A:1107:G:C2	2.93	0.56
1:A:2030:6MZ:OP2	1:A:2031:A:C8	2.58	0.56
34:a:382:A:C8	34:a:383:A:N3	2.74	0.56
1:A:572:A:OP2	18:R:80:ARG:NH2	2.37	0.56
1:A:1047:G:C2'	1:A:1110:G:N2	2.69	0.56
1:A:1033:U:O2	1:A:2750:A:C6	2.59	0.56
1:A:2298:A:C4	1:A:2321:U:C4	2.94	0.56
1:A:1036:G:O6	1:A:1119:U:O2	2.23	0.55
1:A:708:G:O6	1:A:722:A:C6	2.60	0.55
34:a:417:G:C3'	34:a:418:C:H5'	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:472:U:H2'	34:a:473:U:C6	2.42	0.55
1:A:413:C:HO2'	1:A:1880:U:HO2'	1.50	0.55
1:A:1450:G:N2	1:A:1452:G:O6	2.37	0.55
34:a:946:A:H2'	34:a:947:G:C8	2.41	0.55
1:A:272:A:C2	1:A:366:C:N3	2.75	0.55
1:A:1021:A:N3	1:A:1022:G:H5''	2.21	0.55
1:A:2471:A:C2	1:A:2478:A:N6	2.74	0.55
1:A:285:G:H2'	1:A:286:U:O4'	2.07	0.55
1:A:1472:C:C2	1:A:1519:G:O6	2.58	0.55
1:A:1932:A:H2'	1:A:1933:G:O4'	2.06	0.55
34:a:602:A:H2'	34:a:603:U:C6	2.42	0.55
1:A:1051:G:O6	1:A:1109:C:O2	2.24	0.55
34:a:62:U:O2'	34:a:379:C:O2'	2.13	0.55
34:a:182:A:C6	34:a:185:U:O4	2.51	0.55
34:a:632:U:C3'	34:a:633:G:H5''	2.36	0.55
1:A:710:U:N3	1:A:711:G:C8	2.75	0.55
1:A:1795:C:H2'	1:A:1796:U:O4'	2.06	0.55
15:O:51:ALA:HB3	15:O:78:VAL:HG22	1.89	0.55
1:A:362:A:H2'	1:A:363:G:O4'	2.07	0.55
1:A:861:A:N3	2:B:79:G:O2'	2.36	0.55
1:A:1528:A:N6	1:A:1543:G:O2'	2.40	0.55
34:a:138:G:O6	34:a:225:C:N3	2.40	0.55
38:e:110:MET:HE2	38:e:124:ALA:HB1	1.89	0.55
39:f:26:THR:HG22	39:f:36:ILE:CD1	2.37	0.55
1:A:2273:A:H2'	1:A:2274:A:C8	2.42	0.55
11:K:19:VAL:HB	11:K:41:ILE:HG23	1.88	0.55
34:a:141:G:O2'	34:a:142:G:O5'	2.25	0.55
1:A:2287:A:N1	1:A:2346:A:N7	2.55	0.54
34:a:876:C:H1'	41:h:11:THR:HG21	1.88	0.54
57:y:29:G:N2	57:y:41:C:C2	2.75	0.54
1:A:528:A:C2	1:A:2042:A:H2'	2.43	0.54
34:a:602:A:N1	34:a:636:U:O2	2.40	0.54
51:r:10:CYS:SG	51:r:11:ARG:N	2.73	0.54
55:w:17:C:H5'	55:w:117:U:H5''	1.89	0.54
1:A:1182:G:H2'	1:A:1183:U:O4'	2.08	0.54
1:A:2472:G:C2	1:A:2475:C:C2	2.95	0.54
3:C:153:LEU:HD13	3:C:175:LEU:HD21	1.89	0.54
34:a:42:G:C2	34:a:622:A:N3	2.75	0.54
1:A:1068:G:C2	1:A:1096:A:O4'	2.60	0.54
1:A:2788:C:H2'	1:A:2789:C:C6	2.42	0.54
1:A:2856:A:C2'	1:A:2857:G:H5'	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:MET:HE1	3:C:183:VAL:HG21	1.88	0.54
46:m:3:ILE:HD11	46:m:18:LEU:HD22	1.90	0.54
1:A:160:A:N3	1:A:2208:C:O2'	2.39	0.54
1:A:360:U:O2'	1:A:361:G:O5'	2.17	0.54
1:A:1923:U:H2'	1:A:1924:C:C6	2.43	0.54
1:A:1139:G:H2'	1:A:1140:C:O2	2.08	0.54
34:a:491:G:H2'	34:a:492:C:H5'	1.89	0.54
36:c:174:LEU:HD12	36:c:181:ILE:HD13	1.89	0.54
1:A:283:G:O6	1:A:357:C:C1'	2.53	0.54
1:A:2013:A:C2	1:A:2613:U:O4	2.60	0.54
2:B:75:G:H2'	2:B:76:G:O4'	2.07	0.54
29:2:12:ARG:NE	29:2:44:VAL:HG21	2.22	0.54
34:a:454:G:O6	34:a:478:A:C6	2.61	0.54
34:a:455:G:C2	34:a:478:A:C2	2.96	0.54
1:A:85:G:O6	1:A:98:G:C6	2.61	0.54
1:A:1421:G:N2	1:A:1495:A:N1	2.56	0.54
3:C:5:CYS:SG	3:C:12:ARG:NH1	2.80	0.54
1:A:710:U:C4	1:A:711:G:N7	2.76	0.53
1:A:1014:A:H2'	1:A:1015:U:O4'	2.08	0.53
1:A:1077:A:H5'	9:I:93:ASN:HB2	1.90	0.53
4:D:80:TRP:CD1	4:D:202:ILE:HD11	2.43	0.53
34:a:156:C:H2'	34:a:157:U:O4'	2.08	0.53
34:a:270:A:C6	34:a:271:C:C4	2.96	0.53
38:e:80:LEU:HD22	38:e:146:MET:HE2	1.90	0.53
41:h:77:VAL:HG11	41:h:124:ILE:HD12	1.88	0.53
34:a:447:G:O2'	34:a:487:A:N6	2.42	0.53
34:a:513:C:N3	34:a:538:G:N2	2.55	0.53
1:A:12:U:H2'	1:A:12:U:O2	2.07	0.53
1:A:465:G:H2'	1:A:466:A:C8	2.43	0.53
2:B:101:A:H2'	2:B:102:G:O4'	2.09	0.53
9:I:17:ALA:HB2	9:I:42:ASN:HD21	1.72	0.53
34:a:455:G:N1	34:a:477:C:N4	2.56	0.53
34:a:591:U:C2	34:a:648:A:N6	2.77	0.53
1:A:277:G:N1	1:A:360:U:O2'	2.37	0.53
1:A:1913:A:N1	34:a:1493:A:H2'	2.23	0.53
1:A:2298:A:C5	1:A:2321:U:C4	2.96	0.53
1:A:221:A:N7	1:A:427:U:C5	2.74	0.53
1:A:1054:A:N1	1:A:1106:G:H2'	2.24	0.53
1:A:2074:U:H2'	1:A:2075:U:C6	2.44	0.53
1:A:1068:G:N1	1:A:1095:A:H2'	2.23	0.53
34:a:1476:A:H2'	34:a:1477:U:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2898:U:O2'	10:J:134:ALA:O	2.26	0.53
1:A:1487:U:H2'	1:A:1488:C:O4'	2.09	0.53
19:S:5:ALA:HB3	19:S:54:ALA:HB2	1.90	0.53
55:w:17:C:C6	55:w:117:U:C5	2.94	0.53
1:A:2514:U:H2'	1:A:2515:C:C6	2.44	0.52
39:f:29:ILE:HG21	39:f:64:VAL:CG2	2.39	0.52
42:i:83:THR:HG21	42:i:102:PHE:HB3	1.91	0.52
1:A:848:C:H2'	1:A:849:A:C8	2.44	0.52
34:a:185:U:O4	34:a:192:A:N1	2.42	0.52
34:a:384:G:O2'	34:a:385:C:O4'	2.15	0.52
34:a:1486:G:H2'	34:a:1487:G:O4'	2.10	0.52
6:F:24:VAL:O	6:F:27:VAL:HG12	2.09	0.52
34:a:390:U:O2'	49:p:28:ARG:NH2	2.42	0.52
1:A:1050:A:C5	1:A:2751:G:C5	2.97	0.52
40:g:78:ARG:HG2	40:g:83:THR:HG22	1.91	0.52
1:A:1926:U:O2'	1:A:1928:A:N7	2.40	0.52
34:a:132:C:O2	34:a:230:G:N1	2.42	0.52
34:a:378:G:O6	34:a:385:C:N4	2.42	0.52
34:a:708:C:C2'	34:a:709:U:H5'	2.40	0.52
1:A:1129:A:N1	1:A:2569:G:O2'	2.41	0.52
1:A:2812:G:H2'	1:A:2813:A:C8	2.45	0.52
6:F:91:ARG:HA	6:F:95:MET:HB2	1.91	0.52
1:A:1076:C:H2'	1:A:1076:C:O2	2.10	0.52
1:A:2291:U:O2'	1:A:2374:C:O2'	2.11	0.52
19:S:24:ILE:HD11	19:S:36:LEU:HG	1.92	0.52
1:A:1809:A:H2'	1:A:1810:A:C8	2.45	0.52
34:a:36:C:H2'	34:a:37:U:O4'	2.10	0.52
34:a:602:A:N6	34:a:636:U:N3	2.58	0.52
52:s:10:ILE:HD12	52:s:40:PHE:CE2	2.45	0.52
1:A:629:G:H5''	1:A:650:C:O2'	2.10	0.52
34:a:263:A:C2'	34:a:264:C:O2	2.58	0.52
34:a:69:G:H2'	34:a:69:G:N3	2.24	0.51
34:a:459:A:H2'	34:a:460:A:O4'	2.10	0.51
34:a:491:G:H2'	34:a:492:C:C5'	2.40	0.51
1:A:2346:A:H3'	1:A:2347:C:C5'	2.39	0.51
1:A:1052:C:C2	1:A:1107:G:N1	2.77	0.51
1:A:2327:A:H2'	1:A:2328:A:C8	2.46	0.51
13:M:105:MET:HG3	13:M:117:PHE:CZ	2.45	0.51
34:a:849:G:O6	64:a:2001:HOH:O	2.19	0.51
1:A:358:U:C4	1:A:359:G:H1'	2.46	0.51
1:A:987:C:O2'	1:A:1000:A:N3	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:THR:HG23	3:C:176:ARG:HG3	1.92	0.51
34:a:137:U:O2	34:a:226:G:O6	2.29	0.51
51:r:31:TYR:HB3	51:r:54:LEU:HD21	1.93	0.51
1:A:363:G:C6	1:A:364:C:C4	2.99	0.51
1:A:2470:G:C5	1:A:2481:G:N2	2.79	0.51
34:a:415:A:N7	34:a:428:G:O6	2.43	0.51
1:A:709:U:C4	1:A:710:U:C4	2.98	0.51
34:a:827:U:O4	34:a:872:A:C2	2.60	0.51
50:q:22:VAL:HG11	50:q:60:ILE:HD11	1.93	0.51
1:A:273:G:N7	1:A:364:C:C4	2.78	0.51
34:a:257:G:C6	34:a:258:G:C5	2.99	0.51
38:e:93:VAL:HG13	38:e:110:MET:HE3	1.93	0.51
1:A:289:G:C6	1:A:351:C:N3	2.79	0.51
34:a:42:G:N3	34:a:622:A:H2	2.04	0.51
34:a:632:U:H3'	34:a:633:G:H5''	1.93	0.51
2:B:54:G:H2'	2:B:55:U:O4'	2.11	0.51
34:a:488:C:H2'	34:a:489:C:C6	2.46	0.51
1:A:1135:C:H3'	1:A:1136:G:H5'	1.93	0.50
1:A:1483:G:N1	1:A:1507:C:N3	2.58	0.50
17:Q:35:PHE:CZ	17:Q:39:ILE:HD11	2.45	0.50
34:a:626:G:OP1	49:p:18:GLN:NE2	2.44	0.50
1:A:270:A:N6	1:A:369:U:O2'	2.39	0.50
1:A:273:G:N7	1:A:364:C:N4	2.59	0.50
1:A:1533:C:O2	1:A:1538:G:N2	2.44	0.50
34:a:976:G:C8	34:a:1358:U:O2	2.64	0.50
1:A:541:A:H2'	1:A:542:U:O4'	2.12	0.50
1:A:940:G:H5''	1:A:941:A:OP2	2.12	0.50
34:a:1434:A:H2'	34:a:1435:G:O4'	2.11	0.50
58:z:26:THR:OG1	63:z:402:GTP:C5'	2.59	0.50
1:A:2101:A:N6	1:A:2188:U:N3	2.59	0.50
34:a:72:A:C6	34:a:73:C:C6	2.99	0.50
34:a:1448:C:O2	34:a:1448:C:H2'	2.12	0.50
36:c:96:VAL:HB	36:c:97:PRO:HD3	1.94	0.50
63:z:402:GTP:C8	63:z:402:GTP:C5'	2.86	0.50
1:A:804:A:H2'	1:A:806:C:C4	2.46	0.50
1:A:948:C:O2	1:A:984:A:O2'	2.28	0.50
1:A:2013:A:H61	1:A:2613:U:H3	1.57	0.50
39:f:38:ARG:HD2	39:f:63:ASN:CG	2.35	0.50
1:A:1394:U:H4'	1:A:1603:A:H4'	1.93	0.50
1:A:1430:G:H2'	1:A:1431:A:O4'	2.12	0.50
1:A:547:A:H3'	1:A:547:A:N3	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:G:C6	1:A:712:G:C5	2.99	0.50
1:A:2520:C:C6	1:A:2567:G:H1'	2.47	0.50
34:a:382:A:C5	34:a:383:A:N1	2.80	0.50
34:a:6:G:O6	38:e:99:SER:N	2.45	0.50
1:A:1482:G:O2'	1:A:1509:A:N1	2.38	0.49
32:5:87:GLU:HG2	32:5:95:LEU:HD12	1.93	0.49
34:a:197:A:N1	34:a:220:G:O2'	2.44	0.49
34:a:1258:G:H2'	34:a:1259:C:C6	2.47	0.49
1:A:272:A:C2	1:A:365:U:C4	2.99	0.49
1:A:573:U:O4	1:A:2029:G:O2'	2.30	0.49
34:a:1457:G:H2'	34:a:1458:G:O4'	2.13	0.49
1:A:709:U:O4	1:A:722:A:C6	2.65	0.49
8:H:90:LEU:CD2	8:H:94:ILE:HD11	2.42	0.49
34:a:17:U:H2'	34:a:18:C:C6	2.46	0.49
34:a:75:G:N2	34:a:96:U:C4	2.79	0.49
39:f:38:ARG:CD	39:f:63:ASN:HB3	2.39	0.49
58:z:175:LEU:HD12	63:z:402:GTP:C2	2.47	0.49
1:A:1047:G:H2'	1:A:1110:G:C2	2.46	0.49
1:A:1090:A:H61	1:A:1101:U:H3	1.61	0.49
34:a:501:C:O2'	34:a:502:A:OP2	2.23	0.49
36:c:174:LEU:HD11	36:c:200:TRP:CD1	2.47	0.49
49:p:21:VAL:HG21	49:p:60:TRP:CD1	2.47	0.49
1:A:1032:A:H1'	31:4:23:ILE:HD13	1.94	0.49
34:a:692:U:O2'	34:a:694:A:N7	2.39	0.49
45:l:79:ILE:HD12	45:l:96:THR:HG22	1.94	0.49
57:y:27:G:N2	57:y:28:G:H1'	2.28	0.49
1:A:242:G:O2'	1:A:254:G:O6	2.29	0.49
2:B:22:U:H2'	2:B:23:G:H5'	1.94	0.49
34:a:1235:U:H2'	34:a:1236:A:O4'	2.13	0.49
34:a:1305:G:O2'	34:a:1306:A:OP2	2.25	0.49
1:A:2474:U:H3'	1:A:2475:C:C6	2.46	0.49
3:C:90:ILE:HD12	3:C:102:TYR:CD1	2.48	0.49
58:z:98:MET:HE3	58:z:101:ALA:HB2	1.95	0.49
34:a:141:G:C6	34:a:223:A:C6	3.01	0.49
36:c:148:ILE:O	36:c:148:ILE:HG23	2.13	0.49
1:A:724:U:H2'	1:A:725:G:C8	2.47	0.49
1:A:1076:C:N4	9:I:89:SER:OG	2.45	0.49
1:A:1171:G:C8	1:A:1172:C:H1'	2.48	0.49
1:A:1361:G:H2'	1:A:1362:C:C6	2.48	0.49
1:A:2474:U:H2'	1:A:2474:U:O2	2.11	0.49
34:a:299:G:H2'	34:a:300:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:C:O2'	1:A:346:A:N3	2.43	0.49
1:A:570:G:H2'	1:A:2030:6MZ:N7	2.28	0.49
4:D:25:THR:HG21	4:D:193:VAL:HG22	1.94	0.49
14:N:96:ARG:NH1	14:N:116:VAL:HG13	2.28	0.49
25:Y:2:LYS:HD2	25:Y:56:LEU:HD11	1.94	0.49
34:a:138:G:H2'	34:a:139:A:O4'	2.13	0.49
34:a:529:G:O6	45:l:45:ASN:HA	2.13	0.49
34:a:2:A:C2	34:a:614:C:O4'	2.66	0.48
34:a:479:U:H2'	34:a:480:U:H5'	1.94	0.48
34:a:620:C:H2'	34:a:621:A:O4'	2.13	0.48
34:a:1356:G:H2'	34:a:1357:A:C8	2.48	0.48
36:c:39:ARG:NH1	36:c:54:ILE:O	2.47	0.48
1:A:272:A:C2	1:A:365:U:O4	2.65	0.48
1:A:1327:A:N6	1:A:1328:A:C2	2.81	0.48
34:a:69:G:N2	34:a:100:G:C6	2.80	0.48
34:a:144:G:O6	34:a:178:C:N3	2.46	0.48
34:a:575:G:O2'	34:a:821:G:H5'	2.12	0.48
34:a:440:C:N3	34:a:497:G:O6	2.47	0.48
34:a:1218:C:H2'	34:a:1219:A:C8	2.49	0.48
1:A:1726:G:H2'	1:A:1727:A:O4'	2.13	0.48
2:B:106:G:H2'	2:B:107:G:O4'	2.13	0.48
5:E:3:LEU:HD13	5:E:120:VAL:HG21	1.94	0.48
15:O:51:ALA:HB3	15:O:78:VAL:CG2	2.43	0.48
34:a:1448:C:N4	34:a:1456:A:N1	2.62	0.48
1:A:900:A:C2	1:A:901:C:N1	2.81	0.48
34:a:411:A:OP2	37:d:30:LYS:NZ	2.42	0.48
34:a:945:G:C2	34:a:946:A:C8	3.02	0.48
1:A:2585:U:O2	1:A:2585:U:O4'	2.32	0.48
34:a:64:G:C2	34:a:67:C:N4	2.81	0.48
34:a:594:U:O2	34:a:646:G:C2	2.66	0.48
1:A:2471:A:H2'	1:A:2472:G:C4'	2.43	0.48
1:A:2472:G:C6	1:A:2475:C:C6	3.01	0.48
1:A:1050:A:N7	1:A:1051:G:C8	2.77	0.48
1:A:2627:G:N2	1:A:2777:G:OP2	2.47	0.48
2:B:105:G:C2'	2:B:106:G:H5'	2.44	0.48
58:z:25:THR:CB	63:z:402:GTP:O1B	2.58	0.48
1:A:1054:A:N1	1:A:1106:G:O2'	2.41	0.48
17:Q:93:ILE:HD13	18:R:4:VAL:HG13	1.96	0.48
34:a:541:G:H2'	34:a:542:G:O4'	2.13	0.48
47:n:93:ILE:HG21	47:n:96:LEU:HD22	1.96	0.48
1:A:2615:U:C2	27:0:3:GLN:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:63:ILE:HG12	13:M:105:MET:HE3	1.95	0.48
34:a:141:G:N3	34:a:141:G:C2'	2.76	0.48
1:A:267:C:N3	1:A:425:G:O6	2.47	0.47
1:A:1055:G:C8	1:A:1106:G:N1	2.81	0.47
1:A:1533:C:O2	1:A:1538:G:C2	2.66	0.47
1:A:2472:G:C6	1:A:2475:C:H2'	2.48	0.47
34:a:211:G:N3	34:a:211:G:H2'	2.29	0.47
34:a:511:C:O2'	37:d:40:HIS:CE1	2.67	0.47
1:A:1050:A:N6	1:A:2751:G:C5	2.81	0.47
1:A:274:C:H2'	1:A:275:C:O4'	2.13	0.47
1:A:1086:A:H2'	1:A:1086:A:N3	2.29	0.47
1:A:1102:C:H2'	1:A:1103:A:O4'	2.14	0.47
1:A:2297:A:C2	1:A:2321:U:C4	3.02	0.47
34:a:481:G:O2'	34:a:483:C:N4	2.47	0.47
34:a:1064:G:O2'	34:a:1190:G:N2	2.47	0.47
23:W:55:LEU:HD12	23:W:76:ILE:HD12	1.97	0.47
34:a:946:A:O2'	34:a:1333:A:N3	2.46	0.47
1:A:1141:U:OP2	10:J:24:THR:HG21	2.14	0.47
1:A:1484:U:H2'	1:A:1485:U:H6	1.76	0.47
34:a:149:A:H2'	34:a:150:U:C6	2.48	0.47
34:a:386:C:H3'	34:a:387:U:C5'	2.45	0.47
34:a:456:A:H2'	34:a:457:G:C1'	2.45	0.47
40:g:85:GLN:CB	40:g:147:ASN:HD22	2.26	0.47
1:A:351:C:N4	1:A:352:A:N6	2.63	0.47
1:A:924:G:C2'	1:A:925:A:H5'	2.44	0.47
1:A:1052:C:N3	1:A:1107:G:C6	2.81	0.47
1:A:2101:A:C6	1:A:2188:U:N3	2.82	0.47
1:A:2686:G:H2'	1:A:2687:U:O4'	2.15	0.47
1:A:1832:C:N4	1:A:1833:C:C4	2.83	0.47
1:A:2472:G:C6	1:A:2475:C:N1	2.83	0.47
34:a:141:G:C8	34:a:223:A:C2	3.02	0.47
34:a:142:G:N2	34:a:222:C:C1'	2.77	0.47
1:A:1479:G:HO2'	1:A:1560:G:HO2'	1.53	0.47
34:a:369:G:C6	34:a:370:C:C4	3.03	0.47
10:J:35:ARG:HB2	10:J:54:ILE:HD11	1.96	0.47
54:u:28:LEU:HD13	54:u:29:ALA:N	2.30	0.47
1:A:861:A:H2'	1:A:862:G:O4'	2.15	0.47
1:A:1508:A:H4'	1:A:1509:A:OP1	2.15	0.47
34:a:94:G:H4'	34:a:95:C:O5'	2.15	0.47
34:a:1449:C:C2	34:a:1455:G:C2	3.03	0.47
38:e:93:VAL:HG13	38:e:110:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:G:HO2'	1:A:295:G:HO2'	1.62	0.46
1:A:1052:C:O2	1:A:1107:G:C2	2.68	0.46
1:A:1469:A:H2'	1:A:1470:A:C8	2.50	0.46
34:a:195:A:H2'	34:a:196:A:C8	2.50	0.46
34:a:512:U:H2'	34:a:513:C:H5''	1.97	0.46
34:a:513:C:N4	34:a:538:G:N1	2.63	0.46
34:a:648:A:N6	34:a:649:A:C2	2.83	0.46
55:v:18:G:C6	55:v:57:A:N6	2.83	0.46
1:A:287:G:N7	1:A:354:A:N6	2.63	0.46
1:A:586:A:N1	1:A:809:G:O2'	2.45	0.46
1:A:1067:A:H1'	57:y:56:C:C1'	2.46	0.46
34:a:694:A:O2'	55:w:38:A:O2'	2.33	0.46
1:A:1533:C:C2	1:A:1538:G:N2	2.84	0.46
1:A:1799:G:N2	1:A:1818:U:O2'	2.49	0.46
2:B:4:C:H2'	2:B:5:U:O4'	2.16	0.46
22:V:2:PHE:HA	22:V:50:MET:HE1	1.96	0.46
34:a:784:A:H2'	34:a:785:G:C8	2.51	0.46
1:A:1021:A:H3'	1:A:1021:A:N3	2.30	0.46
11:K:24:VAL:HG13	11:K:33:ALA:HB2	1.96	0.46
34:a:109:A:C6	34:a:326:G:C6	3.03	0.46
34:a:141:G:N1	34:a:222:C:O2	2.44	0.46
34:a:807:A:H2'	34:a:808:C:O4'	2.16	0.46
1:A:864:G:O2'	1:A:914:G:O6	2.29	0.46
1:A:1570:A:H2'	1:A:1571:A:C8	2.51	0.46
1:A:1599:U:H2'	1:A:1600:C:C6	2.51	0.46
4:D:4:LEU:HD13	4:D:101:PHE:CE2	2.51	0.46
7:G:104:LEU:HD13	7:G:106:LEU:HD11	1.97	0.46
34:a:126:G:OP1	34:a:605:U:O2'	2.33	0.46
34:a:141:G:C5	34:a:223:A:C2	3.03	0.46
34:a:514:C:C4	34:a:515:G:N7	2.84	0.46
1:A:181:A:C2	1:A:182:A:C4	3.03	0.46
1:A:1050:A:C8	1:A:1051:G:N7	2.77	0.46
34:a:74:A:C2	34:a:97:G:C2	3.04	0.46
34:a:223:A:H2'	34:a:224:U:O4'	2.16	0.46
1:A:2472:G:C4	1:A:2475:C:C4	3.03	0.46
1:A:2797:U:H2'	1:A:2797:U:O2	2.16	0.46
34:a:591:U:N3	34:a:648:A:N6	2.64	0.46
34:a:1391:U:H2'	34:a:1392:G:C8	2.50	0.46
1:A:312:G:H2'	1:A:313:G:H5'	1.97	0.46
1:A:468:G:N7	29:2:39:ARG:NH2	2.64	0.46
1:A:1721:G:H2'	1:A:1738:G:N2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2323:G:H2'	1:A:2324:U:O4'	2.16	0.46
14:N:97:ILE:CD1	14:N:113:ILE:HD12	2.46	0.46
33:6:12:ILE:HD12	33:6:32:LEU:HD11	1.98	0.46
34:a:359:G:H2'	34:a:360:G:O4'	2.16	0.46
34:a:518:C:H5	34:a:530:G:O5'	1.99	0.46
1:A:675:A:N3	1:A:2443:C:O2'	2.46	0.46
34:a:366:A:O3'	34:a:394:G:N2	2.49	0.46
34:a:713:G:H2'	34:a:714:G:C8	2.50	0.46
1:A:543:G:H3'	1:A:544:C:C5'	2.46	0.46
1:A:1165:A:N1	1:A:1184:U:O4	2.48	0.46
1:A:1370:C:H2'	1:A:1371:G:O4'	2.15	0.46
1:A:2038:G:H2'	1:A:2039:U:O4'	2.16	0.46
34:a:592:G:N2	34:a:648:A:H1'	2.31	0.46
54:u:9:GLU:HB2	54:u:10:PRO:HD3	1.97	0.46
34:a:414:A:H2'	34:a:415:A:O4'	2.16	0.45
57:y:28:G:O6	57:y:42:C:N3	2.49	0.45
16:P:91:VAL:HG11	16:P:96:LEU:CD2	2.47	0.45
34:a:675:A:H2'	34:a:676:A:O4'	2.16	0.45
1:A:2472:G:C5	1:A:2475:C:C5	3.04	0.45
1:A:2483:C:O2	1:A:2483:C:O4'	2.32	0.45
34:a:141:G:N1	34:a:222:C:C2	2.82	0.45
1:A:580:U:O3'	17:Q:30:VAL:HG13	2.16	0.45
1:A:609:A:H2'	1:A:610:C:O4'	2.17	0.45
1:A:1613:G:N1	1:A:1617:C:O2'	2.41	0.45
1:A:2560:A:H2'	1:A:2561:U:O4'	2.17	0.45
13:M:57:VAL:HG11	13:M:105:MET:HE1	1.99	0.45
1:A:278:A:C6	1:A:361:G:C8	2.99	0.45
17:Q:104:ALA:O	18:R:48:LYS:NZ	2.50	0.45
34:a:376:G:C2	34:a:389:A:C2	3.04	0.45
1:A:811:U:H2'	12:L:21:ARG:HA	1.99	0.45
6:F:30:VAL:HG12	6:F:95:MET:CE	2.47	0.45
34:a:149:A:C1'	34:a:1446:A:H2	2.30	0.45
34:a:410:G:H1'	34:a:433:G:C2	2.52	0.45
34:a:428:G:O4'	34:a:430:A:C8	2.68	0.45
41:h:104:SER:HB2	41:h:125:ILE:HD11	1.99	0.45
1:A:710:U:O2'	1:A:711:G:OP1	2.20	0.45
1:A:2028:U:C4	1:A:2029:G:O6	2.69	0.45
1:A:2070:A:H2'	1:A:2071:A:O4'	2.15	0.45
1:A:2305:U:H5''	6:F:130:GLY:HA3	1.98	0.45
1:A:2472:G:O6	1:A:2475:C:C3'	2.64	0.45
34:a:502:A:C2	34:a:544:G:C2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:A:C2	1:A:172:A:C2	3.05	0.45
1:A:273:G:N7	1:A:364:C:N3	2.64	0.45
1:A:1042:G:N3	1:A:1042:G:H2'	2.31	0.45
1:A:1062:G:N7	1:A:1063:G:N2	2.59	0.45
1:A:1604:C:O2'	1:A:1610:A:N1	2.41	0.45
1:A:2853:C:H5''	1:A:2853:C:H6	1.81	0.45
3:C:75:ALA:HB1	3:C:93:VAL:CG1	2.47	0.45
12:L:91:ASP:O	12:L:125:LEU:HD13	2.17	0.45
34:a:97:G:H2'	34:a:98:A:O4'	2.17	0.45
34:a:264:C:O2'	50:q:65:PRO:O	2.29	0.45
34:a:1448:C:N4	34:a:1455:G:H1	2.15	0.45
39:f:91:ARG:HD2	39:f:92:THR:HG23	1.98	0.45
49:p:4:ILE:HG12	49:p:21:VAL:HG22	1.99	0.45
1:A:1250:G:OP2	12:L:21:ARG:NH2	2.50	0.45
1:A:1447:C:O2'	1:A:1544:A:N3	2.38	0.45
1:A:1915:3TD:O4'	1:A:1915:3TD:C5	2.54	0.45
34:a:386:C:H3'	34:a:387:U:H5'	1.99	0.45
34:a:591:U:N3	34:a:592:G:N7	2.65	0.45
34:a:1127:G:H1'	34:a:1280:A:C6	2.52	0.45
34:a:1456:A:H2'	34:a:1457:G:O4'	2.17	0.45
58:z:84:ALA:HB3	58:z:87:TYR:CD2	2.52	0.45
1:A:568:U:H1'	1:A:2030:6MZ:C9	2.45	0.45
1:A:706:A:H2'	1:A:707:G:O4'	2.17	0.45
1:A:1052:C:O2	1:A:1052:C:C2'	2.63	0.45
1:A:1054:A:C8	1:A:1107:G:N1	2.85	0.45
1:A:1591:A:H2'	1:A:1592:C:O4'	2.17	0.45
1:A:2636:C:H2'	1:A:2637:U:C6	2.52	0.45
34:a:868:C:H2'	34:a:869:G:O4'	2.17	0.45
1:A:900:A:N3	1:A:900:A:C2'	2.80	0.44
1:A:1105:U:N3	1:A:1106:G:H1'	2.27	0.44
1:A:1351:C:H2'	1:A:1352:U:O4'	2.18	0.44
16:P:91:VAL:HG11	16:P:96:LEU:HD21	1.99	0.44
34:a:246:A:H4'	34:a:247:G:OP1	2.17	0.44
58:z:350:VAL:HG13	58:z:356:ILE:HD11	1.98	0.44
1:A:289:G:O6	1:A:351:C:N3	2.49	0.44
1:A:550:C:C4	1:A:551:G:C5	3.04	0.44
1:A:471:A:OP1	5:E:79:ARG:NH2	2.50	0.44
1:A:2539:C:H5'	31:4:3:VAL:HG21	1.99	0.44
34:a:67:C:O2'	34:a:172:A:O4'	2.34	0.44
34:a:455:G:C6	34:a:477:C:N4	2.85	0.44
34:a:812:G:OP1	34:a:902:G:N2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:h:7:ALA:O	41:h:11:THR:HG23	2.17	0.44
1:A:362:A:N7	1:A:363:G:C5	2.86	0.44
1:A:2016:U:H1'	27:0:2:VAL:CG1	2.48	0.44
1:A:2785:C:H2'	1:A:2786:U:O4'	2.17	0.44
1:A:267:C:C4	1:A:425:G:O6	2.71	0.44
1:A:516:C:OP1	27:0:9:ARG:NH1	2.51	0.44
1:A:709:U:N3	1:A:722:A:C2	2.85	0.44
1:A:1047:G:N2	1:A:1110:G:H2'	2.32	0.44
1:A:1867:G:C6	1:A:1874:C:N4	2.85	0.44
1:A:2478:A:OP1	31:4:32:LYS:NZ	2.50	0.44
1:A:2500:U:O2	1:A:2504:PSU:C2	2.71	0.44
1:A:38:A:H2'	1:A:39:G:O4'	2.18	0.44
1:A:155:A:H2'	1:A:156:A:C8	2.52	0.44
1:A:1050:A:N1	1:A:2751:G:N1	2.66	0.44
1:A:1105:U:H3	1:A:1106:G:H1'	1.79	0.44
1:A:1668:A:O2'	1:A:1674:G:N7	2.43	0.44
9:I:89:SER:OG	9:I:90:GLY:N	2.50	0.44
14:N:24:MET:HE1	14:N:40:LYS:HB3	1.99	0.44
34:a:386:C:C3'	34:a:387:U:C5'	2.96	0.44
41:h:11:THR:HG22	41:h:14:ARG:HH12	1.82	0.44
1:A:543:G:C6	1:A:550:C:N4	2.85	0.44
1:A:2880:C:H2'	1:A:2880:C:O2	2.18	0.44
39:f:26:THR:HG22	39:f:36:ILE:HD13	1.99	0.44
1:A:244:A:H2'	1:A:245:G:O4'	2.18	0.44
1:A:312:G:C2'	1:A:313:G:H5'	2.47	0.44
1:A:958:U:H2'	2:B:89:U:C2	2.53	0.44
6:F:107:VAL:N	6:F:108:PRO:HD2	2.33	0.44
34:a:220:G:H2'	34:a:221:C:C6	2.53	0.44
34:a:757:U:O2'	34:a:879:C:H1'	2.17	0.44
34:a:939:G:OP1	40:g:101:ARG:NH2	2.47	0.44
34:a:1508:A:H2'	34:a:1509:C:O4'	2.18	0.44
1:A:362:A:C5	1:A:363:G:C5	3.05	0.44
1:A:964:C:O2'	1:A:2273:A:N3	2.48	0.44
1:A:1104:C:O2	1:A:1104:C:H2'	2.18	0.44
34:a:663:A:H2'	34:a:664:G:O4'	2.18	0.44
1:A:1176:U:H2'	1:A:1177:G:C8	2.53	0.43
1:A:1414:C:H2'	1:A:1415:U:O4'	2.18	0.43
34:a:69:G:C2	34:a:71:A:C6	3.06	0.43
34:a:404:G:N2	34:a:498:A:C2	2.85	0.43
41:h:105:THR:HB	41:h:120:LEU:HD13	1.99	0.43
1:A:309:A:N3	1:A:329:G:O2'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:G:H3'	12:L:128:THR:HG21	2.00	0.43
1:A:1055:G:C5	1:A:1106:G:C6	3.06	0.43
1:A:2607:G:H2'	1:A:2608:G:O4'	2.18	0.43
2:B:20:G:H2'	2:B:21:G:O4'	2.18	0.43
34:a:71:A:N3	34:a:71:A:H2'	2.34	0.43
34:a:767:A:H2'	34:a:768:A:O4'	2.17	0.43
38:e:108:GLY:O	38:e:109:ALA:HB3	2.18	0.43
1:A:879:G:O6	1:A:898:C:N3	2.52	0.43
1:A:1230:A:H2'	1:A:1231:U:O4'	2.18	0.43
1:A:1268:A:H2'	1:A:1269:A:O4'	2.18	0.43
1:A:2063:C:C5	1:A:2064:C:C5	3.06	0.43
1:A:2078:C:H2'	1:A:2079:U:O4'	2.18	0.43
13:M:53:MET:HG3	13:M:120:ALA:HB2	2.00	0.43
34:a:393:A:N3	34:a:394:G:C8	2.87	0.43
1:A:1028:A:N3	1:A:2486:C:O2'	2.39	0.43
1:A:1131:G:OP1	10:J:82:GLY:HA2	2.18	0.43
1:A:1642:G:H2'	1:A:1643:G:O4'	2.19	0.43
1:A:940:G:H3'	1:A:941:A:H5''	2.00	0.43
1:A:993:G:N3	18:R:91:GLN:NE2	2.66	0.43
1:A:1432:G:H2'	1:A:1433:A:C8	2.53	0.43
11:K:34:GLY:O	11:K:36:GLY:N	2.51	0.43
20:T:61:LEU:HG	20:T:82:LYS:HG2	2.01	0.43
34:a:522:C:H5''	45:I:116:TYR:OH	2.18	0.43
54:u:11:PHE:CZ	54:u:13:VAL:HG13	2.54	0.43
1:A:158:U:O2	1:A:158:U:H2'	2.18	0.43
1:A:363:G:C6	1:A:364:C:N4	2.87	0.43
1:A:725:G:C6	1:A:726:G:N1	2.86	0.43
1:A:1483:G:C2	1:A:1484:U:C4	3.06	0.43
1:A:1483:G:O6	1:A:1508:A:N1	2.52	0.43
1:A:1538:G:C2'	1:A:1539:U:O4'	2.65	0.43
1:A:2477:U:O2	31:4:4:ARG:NH2	2.49	0.43
9:I:27:LEU:HD21	9:I:37:PHE:CD2	2.54	0.43
34:a:141:G:O6	34:a:222:C:N3	2.46	0.43
34:a:456:A:H2'	34:a:457:G:C8	2.53	0.43
34:a:457:G:C2	34:a:458:U:H1'	2.53	0.43
34:a:945:G:H2'	34:a:945:G:N3	2.34	0.43
43:j:57:VAL:HG12	43:j:58:ASN:N	2.33	0.43
1:A:212:G:H2'	1:A:213:A:O4'	2.19	0.43
1:A:281:C:C4	1:A:282:A:N7	2.87	0.43
1:A:1874:C:H2'	1:A:1874:C:O2	2.18	0.43
22:V:4:ILE:HD13	22:V:47:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:154:U:H2'	34:a:155:A:O4'	2.19	0.43
34:a:380:G:N3	34:a:384:G:O6	2.52	0.43
34:a:433:G:H4'	34:a:433:G:OP1	2.17	0.43
38:e:33:THR:HG22	38:e:51:LYS:HG3	2.00	0.43
1:A:1619:G:C8	1:A:1619:G:O5'	2.72	0.43
1:A:2025:C:H2'	1:A:2026:U:C6	2.54	0.43
1:A:2774:C:H2'	1:A:2775:G:O4'	2.19	0.43
13:M:50:ARG:HD3	13:M:65:ILE:HD11	1.99	0.43
32:5:64:VAL:HG12	32:5:64:VAL:O	2.19	0.43
34:a:648:A:N6	34:a:649:A:N1	2.67	0.43
36:c:9:ILE:HD12	47:n:98:LYS:HD3	2.01	0.43
1:A:2029:G:H2'	1:A:2031:A:OP1	2.18	0.43
1:A:2472:G:C4	1:A:2475:C:N3	2.87	0.43
1:A:2852:G:H2'	1:A:2853:C:O4'	2.17	0.43
2:B:4:C:C4	2:B:116:G:O6	2.66	0.43
34:a:953:G:H2'	34:a:954:G:O4'	2.19	0.43
58:z:26:THR:OG1	63:z:402:GTP:H5'	2.19	0.43
1:A:1246:A:H2'	1:A:1247:A:O4'	2.18	0.43
1:A:1722:A:C2	1:A:1739:A:O4'	2.72	0.43
1:A:2337:G:N3	1:A:2337:G:H2'	2.34	0.43
1:A:2577:A:H5''	1:A:2578:G:H5'	2.01	0.43
2:B:90:C:H2'	2:B:91:C:O4'	2.18	0.43
9:I:17:ALA:CB	9:I:42:ASN:HD21	2.32	0.43
34:a:839:C:N3	34:a:847:G:C6	2.87	0.43
34:a:1263:C:C4	34:a:1264:U:C4	3.07	0.43
49:p:2:VAL:HG23	49:p:65:ALA:HB2	2.01	0.43
1:A:14:A:C6	1:A:526:A:C2	3.07	0.42
34:a:195:A:N3	34:a:222:C:O2'	2.51	0.42
34:a:532:A:N6	34:a:1206:G:O2'	2.52	0.42
35:b:169:HIS:CE1	35:b:170:ILE:HG23	2.54	0.42
1:A:534:U:H2'	1:A:535:G:H5''	2.01	0.42
1:A:538:A:H2'	1:A:539:G:O4'	2.18	0.42
1:A:1477:A:N6	1:A:1514:G:O2'	2.51	0.42
1:A:1999:C:H2'	1:A:2000:C:O4'	2.19	0.42
1:A:2471:A:N1	1:A:2479:U:O4	2.51	0.42
18:R:14:VAL:HG21	18:R:98:ILE:HG13	2.01	0.42
26:Z:23:LEU:HD11	26:Z:53:MET:CE	2.49	0.42
34:a:140:U:H2'	34:a:141:G:H5'	2.01	0.42
34:a:778:G:H2'	34:a:779:C:O4'	2.19	0.42
1:A:283:G:H2'	1:A:284:U:O4'	2.19	0.42
1:A:287:G:C5	1:A:354:A:N6	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1090:A:C6	1:A:1102:C:C2	3.07	0.42
1:A:1563:U:H2'	1:A:1564:C:C6	2.55	0.42
2:B:23:G:C6	2:B:24:G:O6	2.71	0.42
5:E:108:ILE:HB	12:L:1:MET:HE3	2.00	0.42
34:a:408:A:C6	34:a:409:U:C4	3.08	0.42
34:a:977:A:O2'	34:a:979:C:OP2	2.34	0.42
38:e:92:ARG:HB2	38:e:127:TYR:HB2	2.02	0.42
58:z:131:ILE:HD12	58:z:195:LEU:HD23	2.00	0.42
1:A:271:G:N1	1:A:367:G:C6	2.88	0.42
1:A:289:G:O6	1:A:351:C:C4	2.72	0.42
1:A:476:G:N1	1:A:479:A:OP2	2.52	0.42
1:A:807:U:H1'	1:A:2445:2MG:OP1	2.20	0.42
1:A:898:C:H2'	1:A:899:A:C8	2.54	0.42
1:A:1352:U:O2'	1:A:1570:A:N3	2.44	0.42
1:A:1519:G:N3	1:A:1519:G:H2'	2.32	0.42
1:A:1857:G:O2'	1:A:1884:G:N2	2.52	0.42
1:A:2320:U:H4'	1:A:2321:U:H5'	1.98	0.42
1:A:2683:C:N3	1:A:2727:A:O2'	2.52	0.42
34:a:325:A:H2'	34:a:326:G:C8	2.54	0.42
1:A:289:G:O6	1:A:350:G:O6	2.37	0.42
1:A:684:G:C2	1:A:794:A:C2	3.08	0.42
1:A:1055:G:C2	1:A:1105:U:C4	3.07	0.42
1:A:1483:G:C2	1:A:1484:U:C5	3.07	0.42
1:A:1851:U:O3'	55:w:71:C:O2'	2.36	0.42
34:a:141:G:O6	34:a:223:A:C6	2.72	0.42
34:a:456:A:H2'	34:a:457:G:N9	2.34	0.42
34:a:680:C:O2	34:a:711:G:C2	2.72	0.42
34:a:690:G:H2'	34:a:691:G:O4'	2.20	0.42
1:A:805:G:OP2	12:L:41:ARG:HG2	2.18	0.42
1:A:1721:G:C2'	1:A:1739:A:N6	2.82	0.42
1:A:2298:A:N3	1:A:2321:U:C5	2.86	0.42
1:A:2472:G:C5	1:A:2475:C:C4	3.07	0.42
22:V:86:LEU:HD13	22:V:89:ILE:HD11	2.01	0.42
58:z:26:THR:OG1	63:z:402:GTP:H5''	2.20	0.42
1:A:1154:G:OP2	17:Q:57:ARG:NH1	2.52	0.42
34:a:75:G:N3	34:a:97:G:N2	2.67	0.42
34:a:602:A:N6	34:a:636:U:H3	2.18	0.42
34:a:847:G:H2'	34:a:848:C:C6	2.55	0.42
38:e:37:VAL:HG11	38:e:113:VAL:HA	2.02	0.42
43:j:42:LEU:HD11	43:j:73:LEU:HG	2.02	0.42
1:A:544:C:N3	1:A:545:U:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1121:C:H5''	1:A:1121:C:H6	1.84	0.42
1:A:1582:C:O2'	1:A:1585:C:N3	2.52	0.42
34:a:99:C:H1'	34:a:100:G:N7	2.35	0.42
55:w:17:C:C5	55:w:117:U:C4	3.00	0.42
1:A:573:U:O4	1:A:2030:6MZ:H3'	2.20	0.42
1:A:1318:U:H2'	1:A:1319:C:C6	2.54	0.42
10:J:64:VAL:HG21	10:J:89:PHE:CZ	2.55	0.42
34:a:109:A:C6	34:a:327:A:C6	3.08	0.42
34:a:380:G:O2'	34:a:382:A:C2	2.54	0.42
34:a:512:U:C2'	34:a:513:C:H5''	2.50	0.42
1:A:1421:G:C2	1:A:1422:G:C8	3.08	0.42
1:A:2755:C:O3'	1:A:2756:U:O2	2.38	0.42
34:a:57:G:H2'	34:a:58:C:C6	2.54	0.42
34:a:142:G:H2'	34:a:143:A:O4'	2.19	0.42
34:a:544:G:OP2	37:d:62:ARG:NH2	2.53	0.42
34:a:827:U:C2	34:a:874:G:N2	2.88	0.42
37:d:23:GLY:HA2	37:d:108:ALA:HB1	2.02	0.42
51:r:20:ILE:HG21	51:r:54:LEU:HA	2.02	0.42
1:A:565:C:H2'	1:A:566:U:O4'	2.20	0.41
1:A:1019:U:OP1	1:A:1035:U:O2'	2.22	0.41
1:A:1067:A:H1'	57:y:56:C:O4'	2.20	0.41
1:A:1614:A:C2	19:S:93:ALA:HB2	2.55	0.41
3:C:52:HIS:CD2	3:C:218:THR:HA	2.55	0.41
34:a:619:U:O2	37:d:129:VAL:HA	2.20	0.41
1:A:36:G:N3	1:A:450:G:O2'	2.50	0.41
1:A:1041:G:N1	1:A:1042:G:C8	2.88	0.41
1:A:1879:C:H2'	1:A:1880:U:O4'	2.20	0.41
2:B:24:G:N7	2:B:56:G:H2'	2.35	0.41
4:D:186:LEU:HD21	16:P:3:ILE:HG23	2.01	0.41
20:T:31:VAL:HG22	20:T:84:TYR:CD2	2.55	0.41
34:a:50:A:N1	34:a:360:G:O2'	2.45	0.41
34:a:150:U:H2'	34:a:151:A:H8	1.85	0.41
34:a:303:A:H2'	34:a:304:U:O4'	2.20	0.41
34:a:394:G:H2'	34:a:395:C:O4'	2.19	0.41
58:z:177:ALA:CB	58:z:188:ILE:HD12	2.50	0.41
12:L:30:THR:O	12:L:32:GLY:N	2.53	0.41
19:S:108:SER:OG	19:S:109:ASP:N	2.53	0.41
21:U:93:ARG:HB2	21:U:102:ILE:HD12	2.03	0.41
29:2:34:ARG:NH1	29:2:42:LEU:O	2.53	0.41
34:a:518:C:C5	34:a:530:G:C8	3.08	0.41
34:a:605:U:C2	34:a:633:G:C6	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:1087:G:C2	34:a:1099:G:C2	3.08	0.41
47:n:54:ASP:O	47:n:55:SER:CB	2.67	0.41
1:A:833:A:H2'	1:A:834:G:C8	2.55	0.41
1:A:1028:A:N6	1:A:1125:G:H2'	2.36	0.41
1:A:1105:U:H2'	1:A:1106:G:H4'	2.01	0.41
1:A:1506:U:N3	1:A:1507:C:N4	2.68	0.41
34:a:75:G:N2	34:a:97:G:N1	2.69	0.41
34:a:75:G:C2	34:a:96:U:C4	3.08	0.41
34:a:256:U:C2	34:a:257:G:N7	2.88	0.41
34:a:890:G:O2'	34:a:906:A:N6	2.53	0.41
57:y:28:G:N1	57:y:42:C:O2	2.51	0.41
1:A:1103:A:C8	1:A:1104:C:C6	3.09	0.41
1:A:1537:G:H3'	1:A:1538:G:C5'	2.50	0.41
1:A:2102:G:C6	1:A:2188:U:C4	3.08	0.41
1:A:2539:C:C5'	31:4:3:VAL:HG21	2.50	0.41
2:B:52:A:N6	15:O:64:TYR:OH	2.51	0.41
2:B:62:C:H2'	2:B:63:C:C6	2.56	0.41
26:Z:23:LEU:HD11	26:Z:53:MET:HE2	2.03	0.41
34:a:455:G:C2	34:a:477:C:N3	2.88	0.41
34:a:622:A:C8	34:a:623:C:C5	3.08	0.41
34:a:1202:U:N3	47:n:82:ILE:HG21	2.36	0.41
48:o:44:GLU:HG2	48:o:45:HIS:CD2	2.56	0.41
1:A:690:G:H2'	1:A:691:C:O4'	2.20	0.41
1:A:1969:A:O2'	1:A:1972:G:N3	2.41	0.41
29:2:34:ARG:HB2	29:2:42:LEU:HD12	2.01	0.41
41:h:10:LEU:HD22	41:h:74:ILE:CD1	2.49	0.41
46:m:94:LEU:HD22	46:m:101:THR:HG21	2.03	0.41
53:t:66:ILE:HG23	53:t:70:LYS:HD2	2.02	0.41
10:J:4:PHE:O	17:Q:63:ARG:NH2	2.52	0.41
34:a:258:G:C6	34:a:259:G:C5	3.09	0.41
34:a:352:C:O2	34:a:352:C:H2'	2.20	0.41
34:a:455:G:N2	34:a:478:A:C2	2.89	0.41
34:a:978:A:O4'	34:a:1322:C:O2	2.39	0.41
36:c:172:VAL:HG12	36:c:174:LEU:HD13	2.03	0.41
38:e:15:ILE:HD13	38:e:37:VAL:HG23	2.01	0.41
39:f:38:ARG:CD	39:f:63:ASN:ND2	2.82	0.41
41:h:24:VAL:HG21	41:h:62:LEU:HD11	2.02	0.41
1:A:742:A:H2'	1:A:743:A:C8	2.56	0.41
1:A:2202:U:O2'	1:A:2204:G:OP1	2.32	0.41
18:R:5:PHE:HB3	18:R:59:ILE:HD12	2.02	0.41
34:a:270:A:H2'	34:a:271:C:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:C:H2'	1:A:226:A:O4'	2.20	0.41
1:A:340:A:H2'	1:A:341:C:O4'	2.20	0.41
1:A:550:C:C4	1:A:551:G:N7	2.89	0.41
1:A:1063:G:O6	1:A:1076:C:N4	2.53	0.41
1:A:1412:U:O4	1:A:1413:A:N6	2.54	0.41
1:A:1502:A:H2'	1:A:1503:A:O4'	2.21	0.41
1:A:1555:G:H5'	1:A:1555:G:C8	2.56	0.41
1:A:1794:A:H2'	1:A:1795:C:C6	2.55	0.41
9:I:32:VAL:HG21	9:I:60:VAL:HG22	2.03	0.41
29:2:44:VAL:O	29:2:44:VAL:HG13	2.21	0.41
34:a:93:U:H3'	34:a:95:C:C5	2.55	0.41
34:a:142:G:C2	34:a:222:C:C1'	3.04	0.41
34:a:144:G:N1	34:a:178:C:O2	2.53	0.41
46:m:15:VAL:HG23	46:m:16:ILE:CD1	2.37	0.41
50:q:11:VAL:HG21	50:q:20:ILE:HD11	2.02	0.41
1:A:1792:G:O2'	1:A:1830:C:OP1	2.36	0.41
1:A:1857:G:N2	1:A:1884:G:O2'	2.41	0.41
8:H:125:THR:HG21	8:H:148:ALA:HB2	2.03	0.41
32:5:48:ALA:HB3	32:5:51:TYR:HE2	1.86	0.41
34:a:622:A:C8	34:a:623:C:C6	3.09	0.41
34:a:1082:A:H2'	34:a:1083:U:O4'	2.21	0.41
47:n:7:ALA:O	47:n:10:VAL:HG12	2.21	0.41
1:A:1049:C:N4	1:A:1050:A:N1	2.68	0.40
1:A:2356:U:H4'	23:W:16:ARG:HG3	2.03	0.40
34:a:602:A:C2	34:a:636:U:O2	2.75	0.40
35:b:27:LYS:N	35:b:28:PRO:CD	2.83	0.40
48:o:77:TYR:CE1	48:o:81:ILE:HD11	2.56	0.40
55:w:16:C:H5''	55:w:17:C:P	2.61	0.40
58:z:98:MET:CE	58:z:101:ALA:HB2	2.51	0.40
1:A:278:A:N7	1:A:362:A:H1'	2.35	0.40
1:A:754:U:H1'	1:A:1618:6MZ:H2	2.02	0.40
1:A:1939:5MU:OP1	1:A:2604:PSU:O2'	2.39	0.40
1:A:2570:G:H2'	1:A:2571:U:O4'	2.22	0.40
1:A:2751:G:H21	7:G:2:ARG:HD3	1.85	0.40
3:C:143:VAL:HB	3:C:153:LEU:HB2	2.03	0.40
34:a:1051:C:O2	34:a:1207:2MG:HM22	2.21	0.40
46:m:89:ARG:HG2	46:m:96:VAL:HA	2.02	0.40
1:A:713:G:N2	1:A:718:A:C5	2.86	0.40
1:A:817:C:H2'	1:A:818:G:O4'	2.22	0.40
1:A:2246:G:H2'	1:A:2247:A:C8	2.57	0.40
1:A:2620:C:H2'	1:A:2621:G:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:78:A:H2'	34:a:79:G:O4'	2.21	0.40
34:a:1448:C:N4	34:a:1456:A:C2	2.90	0.40
1:A:191:A:H2'	1:A:192:C:C6	2.56	0.40
1:A:1020:A:H61	1:A:1141:U:HO2'	1.67	0.40
4:D:80:TRP:HD1	4:D:202:ILE:HD11	1.87	0.40
15:O:92:PHE:HB2	15:O:117:PHE:CE1	2.56	0.40
34:a:130:A:N1	34:a:233:C:H1'	2.36	0.40
34:a:340:U:C2'	34:a:341:C:OP1	2.69	0.40
34:a:652:U:C4	34:a:752:G:N3	2.89	0.40
34:a:687:A:H2'	34:a:701:U:O4	2.21	0.40
34:a:789:U:O2'	34:a:791:G:N7	2.44	0.40
34:a:1305:G:N2	34:a:1331:G:H1'	2.37	0.40
34:a:1518:MA6:H92	34:a:1519:MA6:C9	2.51	0.40
39:f:22:ILE:O	39:f:26:THR:HG23	2.21	0.40
1:A:207:A:H2'	1:A:208:C:O4'	2.22	0.40
1:A:590:A:H2'	1:A:591:U:O4'	2.21	0.40
1:A:735:A:C8	1:A:736:C:C5	3.10	0.40
1:A:756:A:H2'	1:A:757:G:O4'	2.21	0.40
1:A:1061:U:O2	1:A:1061:U:H2'	2.21	0.40
1:A:1105:U:H2'	1:A:1106:G:C4'	2.52	0.40
1:A:1107:G:H2'	1:A:1108:U:O4'	2.21	0.40
1:A:2738:A:C2	1:A:2739:U:H1'	2.56	0.40
3:C:139:THR:HG23	3:C:160:TYR:CD2	2.57	0.40
16:P:64:SER:O	16:P:65:ASN:C	2.64	0.40
35:b:203:ASP:OD1	35:b:204:ASP:N	2.55	0.40
50:q:68:LYS:O	50:q:69:THR:OG1	2.30	0.40
51:r:70:THR:OG1	51:r:71:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/271 (99%)	239 (89%)	27 (10%)	3 (1%)	11	43
4	D	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	24	60
5	E	198/200 (99%)	178 (90%)	18 (9%)	2 (1%)	12	45
6	F	175/177 (99%)	157 (90%)	16 (9%)	2 (1%)	11	43
7	G	172/174 (99%)	158 (92%)	14 (8%)	0	100	100
8	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	4	22
9	I	139/141 (99%)	109 (78%)	23 (16%)	7 (5%)	1	10
10	J	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18	53
11	K	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3	17
12	L	141/143 (99%)	117 (83%)	18 (13%)	6 (4%)	2	12
13	M	134/136 (98%)	128 (96%)	5 (4%)	1 (1%)	18	53
14	N	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	7	32
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14	48
16	P	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	14	48
17	Q	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
18	R	100/102 (98%)	85 (85%)	12 (12%)	3 (3%)	3	19
19	S	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	14	48
20	T	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	5	26
21	U	100/102 (98%)	87 (87%)	9 (9%)	4 (4%)	2	14
22	V	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	11	43
23	W	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
25	Y	58/60 (97%)	54 (93%)	3 (5%)	1 (2%)	7	32
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	44 (83%)	8 (15%)	1 (2%)	6	30
28	1	49/51 (96%)	43 (88%)	6 (12%)	0	100	100
29	2	43/45 (96%)	40 (93%)	2 (5%)	1 (2%)	5	25
30	3	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	99 (77%)	21 (16%)	9 (7%)	1	4
33	6	64/66 (97%)	58 (91%)	4 (6%)	2 (3%)	3	19
35	b	216/218 (99%)	186 (86%)	25 (12%)	5 (2%)	5	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	c	204/206 (99%)	183 (90%)	15 (7%)	6 (3%)	3	20
37	d	203/205 (99%)	183 (90%)	17 (8%)	3 (2%)	8	35
38	e	156/157 (99%)	133 (85%)	21 (14%)	2 (1%)	9	38
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2	13
40	g	149/151 (99%)	131 (88%)	11 (7%)	7 (5%)	2	11
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	97 (78%)	24 (19%)	4 (3%)	3	18
43	j	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	1	9
44	k	114/116 (98%)	97 (85%)	11 (10%)	6 (5%)	1	9
45	l	119/121 (98%)	93 (78%)	19 (16%)	7 (6%)	1	7
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	6	31
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	1	10
48	o	86/88 (98%)	79 (92%)	4 (5%)	3 (4%)	3	16
49	p	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	4	23
50	q	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	1	10
51	r	63/65 (97%)	54 (86%)	6 (10%)	3 (5%)	2	11
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	4	24
54	u	63/65 (97%)	41 (65%)	12 (19%)	10 (16%)	0	0
58	z	391/393 (100%)	357 (91%)	22 (6%)	12 (3%)	3	19
All	All	6219/6322 (98%)	5486 (88%)	581 (9%)	152 (2%)	7	24

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	70	LYS
5	E	83	VAL
6	F	11	VAL
11	K	89	ASN
16	P	65	ASN
32	5	123	ILE
36	c	96	VAL
36	c	156	LEU
42	i	90	ASP
43	j	57	VAL

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Mol	Chain	Res	Type
44	k	88	PRO
44	k	94	SER
53	t	39	GLU
54	u	13	VAL
54	u	14	ALA
54	u	37	TYR
5	E	8	ALA
8	H	3	VAL
8	H	122	LEU
9	I	7	TYR
9	I	38	CYS
10	J	81	ILE
12	L	92	LEU
14	N	117	ASP
15	O	66	GLY
18	R	54	VAL
18	R	55	ASP
20	T	37	ASP
32	5	60	LEU
38	e	77	ASN
40	g	20	GLU
40	g	64	ALA
40	g	129	ASN
42	i	57	VAL
42	i	108	ARG
43	j	29	ALA
44	k	51	PHE
44	k	103	GLY
45	l	75	GLU
46	m	7	ASN
47	n	22	LYS
47	n	55	SER
47	n	90	ARG
48	o	2	LEU
51	r	10	CYS
51	r	17	VAL
54	u	9	GLU
54	u	30	GLU
58	z	161	ASP
8	H	15	LEU
8	H	41	LYS
9	I	6	ALA

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Mol	Chain	Res	Type
9	I	64	ARG
11	K	110	GLU
13	M	69	PRO
14	N	59	SER
22	V	58	SER
25	Y	24	GLU
27	0	2	VAL
32	5	48	ALA
32	5	88	HIS
33	6	4	ASP
35	b	63	LYS
35	b	73	ARG
36	c	95	GLY
37	d	191	SER
39	f	33	GLU
42	i	124	PRO
44	k	118	ASN
45	l	42	LYS
45	l	88	ASP
47	n	2	LYS
47	n	38	ASP
50	q	17	GLU
51	r	46	THR
54	u	11	PHE
58	z	249	GLU
3	C	150	GLY
4	D	149	ASN
6	F	20	ASN
9	I	10	LEU
12	L	15	ALA
12	L	29	LYS
12	L	31	GLY
18	R	43	ASN
20	T	38	ALA
21	U	6	ARG
21	U	97	SER
32	5	118	ILE
35	b	151	LYS
36	c	147	GLY
37	d	166	LYS
38	e	93	VAL
39	f	63	ASN

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Mol	Chain	Res	Type
40	g	18	GLY
40	g	19	SER
40	g	112	ASP
43	j	35	GLN
44	k	13	LYS
45	l	46	SER
48	o	13	GLU
50	q	49	ASN
50	q	69	THR
50	q	79	GLU
58	z	332	PHE
9	I	92	PRO
11	K	35	VAL
19	S	65	ASP
29	2	2	LYS
32	5	55	VAL
32	5	113	PHE
35	b	11	ALA
35	b	192	PRO
36	c	144	GLY
37	d	34	GLU
39	f	92	THR
40	g	56	SER
45	l	33	CYS
45	l	77	SER
48	o	45	HIS
49	p	64	GLY
53	t	44	ALA
54	u	12	ASP
54	u	36	PHE
54	u	65	ARG
58	z	9	LYS
58	z	82	PRO
58	z	126	GLY
58	z	137	CYS
58	z	180	GLY
12	L	115	GLU
21	U	75	ALA
32	5	22	ALA
32	5	108	VAL
39	f	56	LYS
43	j	6	ILE

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Mol	Chain	Res	Type
43	j	75	ASP
45	l	2	THR
46	m	102	LYS
49	p	49	GLY
54	u	24	LYS
58	z	2	LYS
58	z	207	ASP
58	z	248	LYS
11	K	93	GLN
12	L	85	VAL
36	c	148	ILE
3	C	168	GLY
58	z	52	ALA
9	I	12	VAL
21	U	38	ILE
33	6	55	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	216/216 (100%)	206 (95%)	10 (5%)	24	58
4	D	163/163 (100%)	153 (94%)	10 (6%)	17	49
5	E	164/164 (100%)	153 (93%)	11 (7%)	15	46
6	F	148/148 (100%)	143 (97%)	5 (3%)	32	66
7	G	135/135 (100%)	133 (98%)	2 (2%)	57	80
8	H	114/114 (100%)	108 (95%)	6 (5%)	20	54
9	I	109/109 (100%)	102 (94%)	7 (6%)	16	48
10	J	115/115 (100%)	112 (97%)	3 (3%)	40	72
11	K	103/103 (100%)	99 (96%)	4 (4%)	28	62
12	L	102/102 (100%)	93 (91%)	9 (9%)	9	35
13	M	109/109 (100%)	108 (99%)	1 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	99/99 (100%)	94 (95%)	5 (5%)	21	55
15	O	86/86 (100%)	85 (99%)	1 (1%)	63	82
16	P	99/99 (100%)	96 (97%)	3 (3%)	36	69
17	Q	88/88 (100%)	84 (96%)	4 (4%)	24	59
18	R	84/84 (100%)	82 (98%)	2 (2%)	43	73
19	S	92/92 (100%)	91 (99%)	1 (1%)	65	83
20	T	79/79 (100%)	76 (96%)	3 (4%)	29	63
21	U	83/83 (100%)	82 (99%)	1 (1%)	63	82
22	V	77/77 (100%)	76 (99%)	1 (1%)	61	81
23	W	57/57 (100%)	56 (98%)	1 (2%)	51	77
24	X	67/67 (100%)	66 (98%)	1 (2%)	57	80
25	Y	55/55 (100%)	54 (98%)	1 (2%)	51	77
26	Z	47/47 (100%)	47 (100%)	0	100	100
27	0	46/46 (100%)	46 (100%)	0	100	100
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	37/37 (100%)	36 (97%)	1 (3%)	39	71
30	3	51/51 (100%)	50 (98%)	1 (2%)	48	76
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	100 (100%)	0	100	100
33	6	59/59 (100%)	58 (98%)	1 (2%)	53	78
35	b	180/180 (100%)	178 (99%)	2 (1%)	65	83
36	c	170/170 (100%)	167 (98%)	3 (2%)	51	77
37	d	172/172 (100%)	167 (97%)	5 (3%)	37	70
38	e	120/119 (101%)	109 (91%)	11 (9%)	8	33
39	f	87/87 (100%)	84 (97%)	3 (3%)	32	66
40	g	124/124 (100%)	120 (97%)	4 (3%)	34	67
41	h	104/104 (100%)	102 (98%)	2 (2%)	50	76
42	i	105/105 (100%)	102 (97%)	3 (3%)	37	70
43	j	86/86 (100%)	85 (99%)	1 (1%)	63	82
44	k	89/89 (100%)	87 (98%)	2 (2%)	45	74
45	l	102/102 (100%)	99 (97%)	3 (3%)	37	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	m	93/93 (100%)	92 (99%)	1 (1%)	65	83
47	n	83/83 (100%)	81 (98%)	2 (2%)	43	73
48	o	76/76 (100%)	74 (97%)	2 (3%)	40	72
49	p	65/65 (100%)	63 (97%)	2 (3%)	35	68
50	q	74/74 (100%)	71 (96%)	3 (4%)	27	61
51	r	56/56 (100%)	52 (93%)	4 (7%)	13	43
52	s	70/70 (100%)	67 (96%)	3 (4%)	26	60
53	t	65/65 (100%)	61 (94%)	4 (6%)	16	49
54	u	55/55 (100%)	53 (96%)	2 (4%)	31	65
58	z	325/325 (100%)	322 (99%)	3 (1%)	70	85
All	All	5165/5164 (100%)	5005 (97%)	160 (3%)	36	68

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	23	LEU
3	C	35	LYS
3	C	69	ASN
3	C	96	LYS
3	C	101	ARG
3	C	110	LYS
3	C	183	VAL
3	C	200	MET
3	C	203	VAL
3	C	249	VAL
4	D	12	THR
4	D	30	GLU
4	D	33	ARG
4	D	39	ASP
4	D	51	THR
4	D	55	LYS
4	D	56	LYS
4	D	151	THR
4	D	189	VAL
4	D	204	LYS
5	E	2	GLU
5	E	57	LYS
5	E	69	ARG

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Mol	Chain	Res	Type
5	E	111	GLU
5	E	117	ARG
5	E	136	GLN
5	E	139	LYS
5	E	144	GLU
5	E	158	PHE
5	E	165	HIS
5	E	188	MET
6	F	11	VAL
6	F	12	VAL
6	F	67	THR
6	F	114	ARG
6	F	135	ILE
7	G	2	ARG
7	G	169	ARG
8	H	77	THR
8	H	96	THR
8	H	122	LEU
8	H	134	VAL
8	H	138	VAL
8	H	145	ASN
9	I	9	LYS
9	I	12	VAL
9	I	30	GLN
9	I	52	LEU
9	I	67	THR
9	I	72	THR
9	I	134	SER
10	J	12	LYS
10	J	81	ILE
10	J	138	GLN
11	K	7	MET
11	K	31	ARG
11	K	52	VAL
11	K	61	VAL
12	L	1	MET
12	L	2	ARG
12	L	3	LEU
12	L	14	LYS
12	L	41	ARG
12	L	60	ARG
12	L	63	LYS

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Mol	Chain	Res	Type
12	L	92	LEU
12	L	125	LEU
13	M	40	ARG
14	N	34	ILE
14	N	46	ARG
14	N	65	LEU
14	N	98	LEU
14	N	118	ARG
15	O	28	VAL
16	P	26	GLU
16	P	47	ILE
16	P	67	GLU
17	Q	8	ILE
17	Q	40	LYS
17	Q	101	ASP
17	Q	108	LEU
18	R	66	HIS
18	R	73	LYS
19	S	29	VAL
20	T	69	ARG
20	T	76	ARG
20	T	91	GLN
21	U	73	ASN
22	V	42	LEU
23	W	8	ASN
24	X	59	ASP
25	Y	2	LYS
29	2	22	MET
30	3	61	LEU
33	6	37	CYS
35	b	99	MET
35	b	122	ASP
36	c	138	GLN
36	c	156	LEU
36	c	174	LEU
37	d	33	ILE
37	d	140	ASP
37	d	158	LEU
37	d	186	GLU
37	d	190	LEU
38	e	11	GLN
38	e	19	ARG

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Mol	Chain	Res	Type
38	e	38	VAL
38	e	45	VAL
38	e	114	LEU
38	e	119	VAL
38	e	121	ASN
38	e	136	VAL
38	e	139	THR
38	e	141	ASP
38	e	146	MET
39	f	38	ARG
39	f	39	LEU
39	f	91	ARG
40	g	11	ILE
40	g	76	SER
40	g	89	GLU
40	g	147	ASN
41	h	41	GLU
41	h	111	THR
42	i	41	GLU
42	i	42	THR
42	i	65	THR
43	j	67	ILE
44	k	28	ASN
44	k	125	LYS
45	l	38	THR
45	l	77	SER
45	l	93	ARG
46	m	89	ARG
47	n	17	ASP
47	n	75	ARG
48	o	17	ASP
48	o	88	ARG
49	p	31	ARG
49	p	34	GLU
50	q	3	LYS
50	q	37	ILE
50	q	52	CYS
51	r	13	THR
51	r	27	THR
51	r	41	SER
51	r	42	ARG
52	s	5	LYS

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Mol	Chain	Res	Type
52	s	6	LYS
52	s	12	LEU
53	t	7	LYS
53	t	42	ASP
53	t	56	ILE
53	t	68	LYS
54	u	31	VAL
54	u	62	GLU
58	z	22	HIS
58	z	179	GLU
58	z	356	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	20	ASN
3	C	59	GLN
3	C	85	ASN
3	C	152	GLN
3	C	259	ASN
5	E	94	GLN
5	E	136	GLN
6	F	80	GLN
6	F	134	GLN
7	G	37	ASN
7	G	103	ASN
8	H	18	GLN
9	I	42	ASN
9	I	104	GLN
9	I	106	GLN
10	J	47	HIS
11	K	3	GLN
12	L	93	ASN
13	M	3	GLN
13	M	13	HIS
14	N	62	ASN
14	N	73	ASN
15	O	100	HIS
15	O	104	GLN
16	P	6	GLN
16	P	11	GLN
17	Q	51	GLN

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Mol	Chain	Res	Type
18	R	6	GLN
18	R	11	GLN
18	R	12	HIS
19	S	102	HIS
20	T	48	GLN
21	U	45	GLN
21	U	53	GLN
21	U	65	GLN
21	U	73	ASN
25	Y	27	ASN
26	Z	8	GLN
31	4	37	GLN
32	5	4	ASN
33	6	61	ASN
33	6	65	ASN
35	b	18	GLN
35	b	23	ASN
35	b	50	ASN
36	c	68	HIS
36	c	122	GLN
36	c	175	HIS
37	d	35	GLN
37	d	39	GLN
37	d	84	ASN
37	d	88	ASN
37	d	151	GLN
37	d	163	GLN
38	e	72	ASN
38	e	131	ASN
39	f	37	HIS
40	g	129	ASN
41	h	3	GLN
42	i	125	GLN
44	k	37	GLN
44	k	39	ASN
44	k	63	GLN
45	l	45	ASN
45	l	111	GLN
46	m	99	GLN
48	o	27	GLN
48	o	34	GLN
49	p	79	ASN

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Mol	Chain	Res	Type
50	q	49	ASN
51	r	51	GLN
53	t	47	GLN
58	z	51	ASN
58	z	273	ASN
58	z	301	HIS
58	z	329	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	830 (28%)	91 (3%)
2	B	119/120 (99%)	46 (38%)	7 (5%)
34	a	1539/1540 (99%)	498 (32%)	0
55	v	76/77 (98%)	24 (31%)	0
55	w	76/77 (98%)	33 (43%)	0
56	x	11/12 (91%)	4 (36%)	0
57	y	75/76 (98%)	31 (41%)	0
All	All	4793/4805 (99%)	1466 (30%)	98 (2%)

All (1466) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	5	A
1	A	10	A
1	A	12	U
1	A	13	A
1	A	15	G
1	A	23	G
1	A	26	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	45	G
1	A	46	G
1	A	52	A
1	A	60	G
1	A	63	A
1	A	71	A

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Mol	Chain	Res	Type
1	A	74	A
1	A	75	G
1	A	76	C
1	A	80	G
1	A	81	G
1	A	85	G
1	A	86	G
1	A	96	C
1	A	100	U
1	A	101	A
1	A	102	U
1	A	103	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	125	A
1	A	126	A
1	A	135	U
1	A	138	U
1	A	139	U
1	A	140	C
1	A	141	G
1	A	146	A
1	A	147	C
1	A	148	U
1	A	149	A
1	A	157	C
1	A	158	U
1	A	159	G
1	A	160	A
1	A	161	A
1	A	162	U
1	A	163	C
1	A	166	U
1	A	170	U
1	A	171	U
1	A	181	A
1	A	196	A
1	A	199	A
1	A	205	G
1	A	215	G
1	A	216	A

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Mol	Chain	Res	Type
1	A	219	A
1	A	221	A
1	A	222	A
1	A	228	C
1	A	229	C
1	A	231	A
1	A	233	A
1	A	242	G
1	A	243	U
1	A	248	G
1	A	249	C
1	A	255	A
1	A	266	G
1	A	267	C
1	A	272	A
1	A	275	C
1	A	276	U
1	A	277	G
1	A	278	A
1	A	280	U
1	A	281	C
1	A	282	A
1	A	283	G
1	A	284	U
1	A	285	G
1	A	287	G
1	A	288	U
1	A	289	G
1	A	291	G
1	A	294	A
1	A	301	G
1	A	302	C
1	A	305	C
1	A	306	U
1	A	311	A
1	A	313	G
1	A	315	G
1	A	317	G
1	A	323	C
1	A	329	G
1	A	330	A
1	A	343	C

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Mol	Chain	Res	Type
1	A	350	G
1	A	351	C
1	A	352	A
1	A	354	A
1	A	357	C
1	A	358	U
1	A	361	G
1	A	362	A
1	A	363	G
1	A	365	U
1	A	366	C
1	A	367	G
1	A	368	A
1	A	369	U
1	A	371	A
1	A	372	G
1	A	383	C
1	A	386	G
1	A	387	U
1	A	390	U
1	A	396	G
1	A	404	A
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	417	C
1	A	420	C
1	A	422	A
1	A	451	U
1	A	455	C
1	A	456	C
1	A	457	A
1	A	459	U
1	A	473	G
1	A	474	G
1	A	479	A
1	A	481	G
1	A	487	C
1	A	491	G
1	A	492	A
1	A	496	G

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Mol	Chain	Res	Type
1	A	503	A
1	A	504	A
1	A	505	A
1	A	509	C
1	A	513	A
1	A	518	G
1	A	526	A
1	A	527	C
1	A	529	A
1	A	532	A
1	A	533	G
1	A	535	G
1	A	542	U
1	A	543	G
1	A	544	C
1	A	545	U
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	550	C
1	A	557	C
1	A	563	A
1	A	573	U
1	A	575	A
1	A	586	A
1	A	603	A
1	A	613	A
1	A	614	A
1	A	615	U
1	A	616	A
1	A	622	G
1	A	627	A
1	A	637	A
1	A	640	C
1	A	644	A
1	A	645	C
1	A	646	U
1	A	647	G
1	A	651	G
1	A	652	U
1	A	653	U

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Mol	Chain	Res	Type
1	A	654	A
1	A	655	A
1	A	656	G
1	A	659	G
1	A	661	A
1	A	668	A
1	A	678	C
1	A	685	A
1	A	686	U
1	A	694	U
1	A	695	G
1	A	696	G
1	A	710	U
1	A	711	G
1	A	713	G
1	A	714	U
1	A	717	C
1	A	730	A
1	A	734	A
1	A	738	G
1	A	747	5MC
1	A	752	A
1	A	763	G
1	A	764	A
1	A	765	C
1	A	771	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	783	A
1	A	784	G
1	A	785	G
1	A	788	A
1	A	805	G
1	A	812	C
1	A	816	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	843	G
1	A	844	A

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Mol	Chain	Res	Type
1	A	845	A
1	A	846	C
1	A	847	U
1	A	858	G
1	A	859	G
1	A	860	U
1	A	866	A
1	A	868	U
1	A	869	G
1	A	870	U
1	A	872	U
1	A	873	C
1	A	877	A
1	A	878	A
1	A	880	G
1	A	882	G
1	A	892	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	C
1	A	903	C
1	A	906	U
1	A	907	G
1	A	909	A
1	A	910	A
1	A	914	G
1	A	915	C
1	A	925	A
1	A	934	U
1	A	935	C
1	A	940	G
1	A	941	A
1	A	946	C
1	A	951	C
1	A	961	C
1	A	968	C
1	A	974	G
1	A	982	C
1	A	983	A
1	A	984	A

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Mol	Chain	Res	Type
1	A	985	C
1	A	989	G
1	A	990	A
1	A	995	C
1	A	996	A
1	A	999	U
1	A	1003	G
1	A	1005	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1019	U
1	A	1020	A
1	A	1021	A
1	A	1022	G
1	A	1023	U
1	A	1025	G
1	A	1026	G
1	A	1033	U
1	A	1042	G
1	A	1043	C
1	A	1044	C
1	A	1045	C
1	A	1046	A
1	A	1047	G
1	A	1049	C
1	A	1050	A
1	A	1051	G
1	A	1052	C
1	A	1053	C
1	A	1054	A
1	A	1055	G
1	A	1057	A
1	A	1059	G
1	A	1060	U
1	A	1061	U
1	A	1062	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1067	A
1	A	1068	G

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Mol	Chain	Res	Type
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1073	A
1	A	1075	C
1	A	1076	C
1	A	1079	C
1	A	1084	A
1	A	1087	G
1	A	1088	A
1	A	1090	A
1	A	1096	A
1	A	1097	U
1	A	1101	U
1	A	1103	A
1	A	1104	C
1	A	1105	U
1	A	1106	G
1	A	1110	G
1	A	1112	G
1	A	1114	C
1	A	1115	G
1	A	1116	G
1	A	1117	C
1	A	1119	U
1	A	1121	C
1	A	1130	U
1	A	1131	G
1	A	1132	U
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1140	C
1	A	1141	U
1	A	1142	A
1	A	1144	A
1	A	1149	G
1	A	1151	A
1	A	1168	G
1	A	1169	A
1	A	1171	G
1	A	1172	C

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Mol	Chain	Res	Type
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1180	U
1	A	1195	G
1	A	1203	U
1	A	1204	A
1	A	1205	A
1	A	1218	G
1	A	1236	G
1	A	1248	G
1	A	1250	G
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1287	A
1	A	1289	C
1	A	1300	G
1	A	1301	A
1	A	1306	C
1	A	1321	A
1	A	1343	G
1	A	1345	C
1	A	1346	G
1	A	1350	C
1	A	1352	U
1	A	1353	A
1	A	1360	G
1	A	1365	A
1	A	1368	G
1	A	1378	A
1	A	1379	U
1	A	1386	C
1	A	1387	A
1	A	1392	A
1	A	1395	A
1	A	1397	U
1	A	1403	A

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Mol	Chain	Res	Type
1	A	1407	G
1	A	1409	U
1	A	1410	G
1	A	1416	G
1	A	1418	G
1	A	1419	A
1	A	1420	A
1	A	1427	A
1	A	1428	C
1	A	1434	A
1	A	1437	C
1	A	1451	C
1	A	1452	G
1	A	1453	A
1	A	1456	G
1	A	1458	U
1	A	1459	G
1	A	1461	C
1	A	1475	G
1	A	1476	U
1	A	1478	G
1	A	1479	G
1	A	1480	C
1	A	1481	U
1	A	1482	G
1	A	1484	U
1	A	1485	U
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1494	A
1	A	1498	C
1	A	1503	A
1	A	1504	A
1	A	1506	U
1	A	1508	A
1	A	1509	A
1	A	1510	G
1	A	1515	A
1	A	1519	G
1	A	1522	A
1	A	1524	G

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Mol	Chain	Res	Type
1	A	1528	A
1	A	1529	G
1	A	1533	C
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1539	U
1	A	1540	G
1	A	1542	U
1	A	1543	G
1	A	1546	G
1	A	1555	G
1	A	1556	C
1	A	1558	C
1	A	1559	U
1	A	1566	A
1	A	1569	A
1	A	1572	A
1	A	1578	U
1	A	1579	A
1	A	1581	G
1	A	1582	C
1	A	1584	U
1	A	1585	C
1	A	1589	U
1	A	1590	A
1	A	1591	A
1	A	1607	C
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1612	C
1	A	1616	A
1	A	1617	C
1	A	1618	6MZ
1	A	1619	G
1	A	1622	G
1	A	1644	C
1	A	1647	U
1	A	1648	U
1	A	1649	G

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Mol	Chain	Res	Type
1	A	1651	G
1	A	1654	A
1	A	1672	A
1	A	1674	G
1	A	1675	C
1	A	1678	A
1	A	1679	A
1	A	1693	U
1	A	1695	G
1	A	1703	G
1	A	1715	G
1	A	1716	U
1	A	1717	A
1	A	1721	G
1	A	1722	A
1	A	1723	G
1	A	1724	G
1	A	1725	C
1	A	1726	G
1	A	1728	C
1	A	1729	U
1	A	1731	G
1	A	1733	U
1	A	1734	C
1	A	1735	G
1	A	1738	G
1	A	1739	A
1	A	1750	G
1	A	1764	C
1	A	1773	A
1	A	1776	G
1	A	1780	A
1	A	1782	U
1	A	1784	A
1	A	1791	A
1	A	1800	C
1	A	1801	A
1	A	1802	A
1	A	1808	A
1	A	1811	G
1	A	1812	U
1	A	1816	C

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Mol	Chain	Res	Type
1	A	1818	U
1	A	1819	A
1	A	1839	G
1	A	1842	G
1	A	1847	G
1	A	1853	A
1	A	1857	G
1	A	1858	A
1	A	1863	G
1	A	1866	A
1	A	1867	G
1	A	1870	C
1	A	1871	A
1	A	1872	A
1	A	1873	G
1	A	1875	G
1	A	1876	A
1	A	1877	A
1	A	1878	G
1	A	1881	C
1	A	1884	G
1	A	1885	A
1	A	1890	A
1	A	1896	G
1	A	1902	C
1	A	1905	C
1	A	1906	G
1	A	1907	G
1	A	1913	A
1	A	1914	C
1	A	1915	3TD
1	A	1916	A
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1939	5MU
1	A	1940	U
1	A	1941	C
1	A	1942	C

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Mol	Chain	Res	Type
1	A	1955	U
1	A	1962	5MC
1	A	1964	G
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1982	U
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2004	G
1	A	2021	C
1	A	2022	U
1	A	2023	C
1	A	2027	G
1	A	2029	G
1	A	2030	6MZ
1	A	2031	A
1	A	2033	A
1	A	2036	C
1	A	2043	C
1	A	2049	G
1	A	2051	A
1	A	2055	C
1	A	2056	G
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2067	G
1	A	2069	7MG
1	A	2072	C
1	A	2077	A
1	A	2080	A
1	A	2092	U
1	A	2093	G
1	A	2095	A
1	A	2097	A
1	A	2098	U

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Mol	Chain	Res	Type
1	A	2099	U
1	A	2100	G
1	A	2106	U
1	A	2108	A
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2118	U
1	A	2119	A
1	A	2121	G
1	A	2127	G
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2141	G
1	A	2145	C
1	A	2147	A
1	A	2157	G
1	A	2162	G
1	A	2164	C
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2186	G
1	A	2189	U
1	A	2190	G
1	A	2191	A
1	A	2192	U
1	A	2193	G
1	A	2194	U
1	A	2198	A
1	A	2199	A
1	A	2204	G
1	A	2211	A
1	A	2214	C
1	A	2220	U
1	A	2223	G
1	A	2225	A
1	A	2226	C
1	A	2238	G

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Mol	Chain	Res	Type
1	A	2239	G
1	A	2246	G
1	A	2263	C
1	A	2267	A
1	A	2268	A
1	A	2278	A
1	A	2283	C
1	A	2286	G
1	A	2287	A
1	A	2292	U
1	A	2293	G
1	A	2295	C
1	A	2296	U
1	A	2297	A
1	A	2302	U
1	A	2305	U
1	A	2307	G
1	A	2309	A
1	A	2311	A
1	A	2315	G
1	A	2319	G
1	A	2321	U
1	A	2322	A
1	A	2325	G
1	A	2326	C
1	A	2327	A
1	A	2331	G
1	A	2333	A
1	A	2336	A
1	A	2337	G
1	A	2345	G
1	A	2347	C
1	A	2350	C
1	A	2352	A
1	A	2357	G
1	A	2361	G
1	A	2373	G
1	A	2377	A
1	A	2378	A
1	A	2383	G
1	A	2385	C
1	A	2391	G

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Mol	Chain	Res	Type
1	A	2392	A
1	A	2396	G
1	A	2402	U
1	A	2403	C
1	A	2404	U
1	A	2406	A
1	A	2407	A
1	A	2408	U
1	A	2409	G
1	A	2410	G
1	A	2414	G
1	A	2423	U
1	A	2424	C
1	A	2429	G
1	A	2430	A
1	A	2435	A
1	A	2436	G
1	A	2441	U
1	A	2445	2MG
1	A	2447	G
1	A	2448	A
1	A	2459	A
1	A	2469	A
1	A	2472	G
1	A	2473	U
1	A	2474	U
1	A	2475	C
1	A	2476	A
1	A	2481	G
1	A	2491	U
1	A	2492	U
1	A	2494	G
1	A	2502	G
1	A	2503	2MA
1	A	2504	PSU
1	A	2505	G
1	A	2506	U
1	A	2517	C
1	A	2518	A
1	A	2523	G
1	A	2529	G
1	A	2530	A

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Mol	Chain	Res	Type
1	A	2535	G
1	A	2547	A
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2574	G
1	A	2577	A
1	A	2585	U
1	A	2586	U
1	A	2602	A
1	A	2609	U
1	A	2610	C
1	A	2613	U
1	A	2623	G
1	A	2624	G
1	A	2629	U
1	A	2636	C
1	A	2647	U
1	A	2649	C
1	A	2654	A
1	A	2656	U
1	A	2668	G
1	A	2669	G
1	A	2671	G
1	A	2685	G
1	A	2689	U
1	A	2690	U
1	A	2692	G
1	A	2702	G
1	A	2707	U
1	A	2708	G
1	A	2713	U
1	A	2714	G
1	A	2718	G
1	A	2721	A
1	A	2722	G
1	A	2724	U
1	A	2726	A
1	A	2729	G
1	A	2732	G

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Mol	Chain	Res	Type
1	A	2739	U
1	A	2740	A
1	A	2744	G
1	A	2748	A
1	A	2753	A
1	A	2758	A
1	A	2759	G
1	A	2761	A
1	A	2764	A
1	A	2765	A
1	A	2769	U
1	A	2771	C
1	A	2778	A
1	A	2782	G
1	A	2783	U
1	A	2784	U
1	A	2790	U
1	A	2791	G
1	A	2793	C
1	A	2796	C
1	A	2798	U
1	A	2799	G
1	A	2801	G
1	A	2803	G
1	A	2806	C
1	A	2809	A
1	A	2818	U
1	A	2820	A
1	A	2821	A
1	A	2835	A
1	A	2837	A
1	A	2845	U
1	A	2849	U
1	A	2850	A
1	A	2853	C
1	A	2857	G
1	A	2859	G
1	A	2861	U
1	A	2867	G
1	A	2868	A
1	A	2872	A
1	A	2873	A

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Mol	Chain	Res	Type
1	A	2874	C
1	A	2879	A
1	A	2880	C
1	A	2881	U
1	A	2883	A
1	A	2884	U
1	A	2886	A
1	A	2891	U
1	A	2894	G
1	A	2897	U
1	A	2900	A
1	A	2901	C
1	A	2902	C
1	A	2903	U
2	B	4	C
2	B	5	U
2	B	6	G
2	B	11	C
2	B	12	C
2	B	13	G
2	B	15	A
2	B	22	U
2	B	23	G
2	B	24	G
2	B	33	G
2	B	34	A
2	B	35	C
2	B	36	C
2	B	40	U
2	B	41	G
2	B	42	C
2	B	44	G
2	B	46	A
2	B	47	C
2	B	51	G
2	B	53	A
2	B	56	G
2	B	57	A
2	B	59	A
2	B	61	G
2	B	64	G
2	B	66	A

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Mol	Chain	Res	Type
2	B	67	G
2	B	70	C
2	B	81	G
2	B	87	U
2	B	88	C
2	B	89	U
2	B	90	C
2	B	91	C
2	B	95	U
2	B	96	G
2	B	100	G
2	B	105	G
2	B	106	G
2	B	109	A
2	B	112	G
2	B	117	G
2	B	118	C
2	B	119	A
34	a	2	A
34	a	3	A
34	a	4	U
34	a	5	U
34	a	6	G
34	a	7	A
34	a	9	G
34	a	10	A
34	a	28	A
34	a	31	G
34	a	32	A
34	a	38	G
34	a	39	G
34	a	41	G
34	a	45	G
34	a	47	C
34	a	48	C
34	a	50	A
34	a	51	A
34	a	61	G
34	a	63	C
34	a	64	G
34	a	66	A
34	a	67	C

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Mol	Chain	Res	Type
34	a	68	G
34	a	69	G
34	a	70	U
34	a	72	A
34	a	73	C
34	a	76	G
34	a	77	A
34	a	78	A
34	a	79	G
34	a	80	A
34	a	83	C
34	a	85	U
34	a	86	G
34	a	87	C
34	a	89	U
34	a	94	G
34	a	95	C
34	a	96	U
34	a	97	G
34	a	98	A
34	a	99	C
34	a	100	G
34	a	102	G
34	a	107	G
34	a	112	G
34	a	115	G
34	a	116	A
34	a	121	U
34	a	122	G
34	a	129	A
34	a	130	A
34	a	131	A
34	a	140	U
34	a	141	G
34	a	142	G
34	a	144	G
34	a	145	G
34	a	146	G
34	a	149	A
34	a	151	A
34	a	152	A
34	a	161	A

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Mol	Chain	Res	Type
34	a	163	C
34	a	164	G
34	a	165	G
34	a	166	U
34	a	169	C
34	a	173	U
34	a	179	A
34	a	181	A
34	a	182	A
34	a	183	C
34	a	184	G
34	a	185	U
34	a	187	G
34	a	188	C
34	a	189	A
34	a	191	G
34	a	193	C
34	a	195	A
34	a	196	A
34	a	197	A
34	a	202	G
34	a	203	G
34	a	207	C
34	a	209	U
34	a	210	C
34	a	211	G
34	a	212	G
34	a	213	G
34	a	215	C
34	a	216	U
34	a	218	U
34	a	222	C
34	a	226	G
34	a	230	G
34	a	232	G
34	a	245	U
34	a	247	G
34	a	248	C
34	a	251	G
34	a	254	G
34	a	255	G
34	a	264	C

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Mol	Chain	Res	Type
34	a	266	G
34	a	267	C
34	a	271	C
34	a	279	A
34	a	280	C
34	a	281	G
34	a	282	A
34	a	289	G
34	a	300	A
34	a	305	G
34	a	306	A
34	a	308	C
34	a	319	G
34	a	321	A
34	a	323	U
34	a	324	G
34	a	328	C
34	a	329	A
34	a	330	C
34	a	331	G
34	a	335	C
34	a	341	C
34	a	343	U
34	a	345	C
34	a	346	G
34	a	349	A
34	a	352	C
34	a	354	G
34	a	366	A
34	a	367	U
34	a	368	U
34	a	370	C
34	a	372	C
34	a	373	A
34	a	376	G
34	a	380	G
34	a	381	C
34	a	382	A
34	a	383	A
34	a	384	G
34	a	385	C
34	a	386	C

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Mol	Chain	Res	Type
34	a	387	U
34	a	388	G
34	a	392	C
34	a	393	A
34	a	394	G
34	a	397	A
34	a	398	U
34	a	404	G
34	a	405	U
34	a	406	G
34	a	411	A
34	a	412	A
34	a	413	G
34	a	414	A
34	a	415	A
34	a	418	C
34	a	420	U
34	a	421	U
34	a	422	C
34	a	424	G
34	a	425	G
34	a	428	G
34	a	429	U
34	a	433	G
34	a	434	U
34	a	435	A
34	a	436	C
34	a	437	U
34	a	439	U
34	a	441	A
34	a	443	C
34	a	445	G
34	a	446	G
34	a	447	G
34	a	449	G
34	a	453	G
34	a	458	U
34	a	464	U
34	a	466	A
34	a	467	U
34	a	468	A
34	a	475	C

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Mol	Chain	Res	Type
34	a	477	C
34	a	480	U
34	a	484	G
34	a	485	U
34	a	486	U
34	a	490	C
34	a	491	G
34	a	492	C
34	a	495	A
34	a	496	A
34	a	497	G
34	a	499	A
34	a	500	G
34	a	509	A
34	a	510	A
34	a	511	C
34	a	513	C
34	a	517	G
34	a	518	C
34	a	520	A
34	a	521	G
34	a	525	C
34	a	527	7MG
34	a	531	U
34	a	542	G
34	a	545	C
34	a	546	A
34	a	547	A
34	a	548	G
34	a	550	G
34	a	572	A
34	a	573	A
34	a	575	G
34	a	576	C
34	a	577	G
34	a	579	A
34	a	594	U
34	a	596	A
34	a	601	G
34	a	602	A
34	a	608	A
34	a	612	C

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Mol	Chain	Res	Type
34	a	613	C
34	a	614	C
34	a	615	G
34	a	617	G
34	a	618	C
34	a	620	C
34	a	621	A
34	a	626	G
34	a	627	G
34	a	628	G
34	a	632	U
34	a	633	G
34	a	635	A
34	a	636	U
34	a	637	C
34	a	639	G
34	a	642	A
34	a	648	A
34	a	652	U
34	a	653	U
34	a	654	G
34	a	659	U
34	a	660	C
34	a	665	A
34	a	671	G
34	a	687	A
34	a	695	A
34	a	700	G
34	a	703	G
34	a	704	A
34	a	709	U
34	a	711	G
34	a	712	A
34	a	713	G
34	a	720	C
34	a	721	G
34	a	722	G
34	a	723	U
34	a	724	G
34	a	731	G
34	a	733	G
34	a	737	C

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Mol	Chain	Res	Type
34	a	742	G
34	a	753	A
34	a	754	C
34	a	755	G
34	a	758	C
34	a	759	A
34	a	769	G
34	a	777	A
34	a	793	U
34	a	794	A
34	a	802	A
34	a	815	A
34	a	817	C
34	a	818	G
34	a	819	A
34	a	821	G
34	a	832	G
34	a	836	G
34	a	840	C
34	a	843	U
34	a	844	G
34	a	846	G
34	a	848	C
34	a	849	G
34	a	852	G
34	a	872	A
34	a	884	U
34	a	885	G
34	a	899	C
34	a	902	G
34	a	914	A
34	a	926	G
34	a	932	C
34	a	934	C
34	a	935	A
34	a	939	G
34	a	951	G
34	a	960	U
34	a	961	U
34	a	966	2MG
34	a	969	A
34	a	971	G

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Mol	Chain	Res	Type
34	a	974	A
34	a	975	A
34	a	976	G
34	a	977	A
34	a	978	A
34	a	982	U
34	a	984	C
34	a	989	U
34	a	991	U
34	a	992	U
34	a	993	G
34	a	998	C
34	a	999	C
34	a	1001	C
34	a	1003	G
34	a	1004	A
34	a	1006	G
34	a	1016	A
34	a	1020	G
34	a	1027	C
34	a	1028	C
34	a	1030	U
34	a	1031	C
34	a	1033	G
34	a	1034	G
34	a	1035	A
34	a	1043	G
34	a	1044	A
34	a	1045	C
34	a	1053	G
34	a	1056	U
34	a	1065	U
34	a	1070	U
34	a	1088	G
34	a	1089	G
34	a	1094	G
34	a	1095	U
34	a	1096	C
34	a	1098	C
34	a	1101	A
34	a	1104	G
34	a	1108	G

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Mol	Chain	Res	Type
34	a	1124	G
34	a	1125	U
34	a	1126	U
34	a	1132	C
34	a	1133	G
34	a	1134	G
34	a	1136	C
34	a	1137	C
34	a	1138	G
34	a	1139	G
34	a	1142	G
34	a	1143	G
34	a	1145	A
34	a	1146	A
34	a	1151	A
34	a	1152	A
34	a	1154	G
34	a	1157	A
34	a	1158	C
34	a	1159	U
34	a	1160	G
34	a	1162	C
34	a	1167	A
34	a	1168	U
34	a	1169	A
34	a	1171	A
34	a	1182	G
34	a	1184	G
34	a	1190	G
34	a	1191	A
34	a	1196	A
34	a	1197	A
34	a	1201	A
34	a	1202	U
34	a	1206	G
34	a	1211	U
34	a	1212	U
34	a	1213	A
34	a	1217	C
34	a	1219	A
34	a	1220	G
34	a	1225	A

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Mol	Chain	Res	Type
34	a	1226	C
34	a	1227	A
34	a	1228	C
34	a	1236	A
34	a	1238	A
34	a	1241	G
34	a	1244	G
34	a	1247	U
34	a	1256	A
34	a	1257	A
34	a	1258	G
34	a	1260	G
34	a	1261	A
34	a	1263	C
34	a	1266	G
34	a	1269	A
34	a	1270	G
34	a	1272	G
34	a	1273	C
34	a	1274	A
34	a	1275	A
34	a	1280	A
34	a	1281	C
34	a	1282	C
34	a	1285	A
34	a	1286	U
34	a	1287	A
34	a	1293	C
34	a	1294	G
34	a	1296	C
34	a	1297	G
34	a	1298	U
34	a	1300	G
34	a	1301	U
34	a	1302	C
34	a	1304	G
34	a	1305	G
34	a	1306	A
34	a	1308	U
34	a	1312	G
34	a	1317	C
34	a	1318	A

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Mol	Chain	Res	Type
34	a	1320	C
34	a	1321	U
34	a	1331	G
34	a	1338	G
34	a	1340	A
34	a	1345	U
34	a	1346	A
34	a	1348	U
34	a	1352	C
34	a	1353	G
34	a	1360	A
34	a	1363	A
34	a	1368	A
34	a	1370	G
34	a	1371	G
34	a	1379	G
34	a	1380	U
34	a	1381	U
34	a	1382	C
34	a	1383	C
34	a	1397	C
34	a	1398	A
34	a	1399	C
34	a	1400	C
34	a	1419	G
34	a	1429	A
34	a	1433	A
34	a	1434	A
34	a	1438	G
34	a	1441	A
34	a	1442	G
34	a	1445	U
34	a	1446	A
34	a	1448	C
34	a	1450	U
34	a	1452	C
34	a	1458	G
34	a	1487	G
34	a	1492	A
34	a	1497	G
34	a	1502	A
34	a	1503	A

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Mol	Chain	Res	Type
34	a	1506	U
34	a	1517	G
34	a	1519	MA6
34	a	1529	G
34	a	1530	G
34	a	1533	C
34	a	1534	A
34	a	1535	C
34	a	1536	C
34	a	1537	U
34	a	1538	C
34	a	1539	C
55	v	4	G
55	v	6	G
55	v	7	4SU
55	v	8	G
55	v	10	A
55	v	13	A
55	v	15	C
55	v	17	U
55	v	18	G
55	v	20	H2U
55	v	21	A
55	v	22	G
55	v	25	C
55	v	31	G
55	v	42	G
55	v	47	U
55	v	52	G
55	v	60	U
55	v	61	C
55	v	66	C
55	v	67	C
55	v	69	C
55	v	73	A
55	v	76	A
55	w	3	C
55	w	5	G
55	w	8	4SU
55	w	9	G
55	w	14	A
55	w	16	C

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Mol	Chain	Res	Type
55	w	17	C
55	w	117	U
55	w	18	G
55	w	19	G
55	w	20	H2U
55	w	21	A
55	w	22	G
55	w	24	U
55	w	25	C
55	w	28	C
55	w	30	G
55	w	34	C
55	w	37	A
55	w	38	A
55	w	42	G
55	w	48	C
55	w	49	G
55	w	56	C
55	w	57	A
55	w	59	A
55	w	67	C
55	w	69	C
55	w	70	G
55	w	71	C
55	w	73	A
55	w	75	C
55	w	76	A
56	x	14	C
56	x	15	U
56	x	23	C
56	x	24	G
57	y	3	C
57	y	4	C
57	y	5	G
57	y	8	4SU
57	y	9	A
57	y	10	G
57	y	11	C
57	y	16	H2U
57	y	17	C
57	y	18	G
57	y	20	H2U

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Mol	Chain	Res	Type
57	y	21	A
57	y	24	G
57	y	28	G
57	y	30	G
57	y	31	A
57	y	33	U
57	y	36	A
57	y	37	MIA
57	y	44	G
57	y	45	U
57	y	46	7MG
57	y	47	U
57	y	48	C
57	y	52	G
57	y	56	C
57	y	59	U
57	y	61	C
57	y	65	G
57	y	75	C
57	y	76	A

All (98) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	51	G
1	A	84	A
1	A	85	G
1	A	101	A
1	A	119	A
1	A	141	G
1	A	162	U
1	A	196	A
1	A	204	A
1	A	242	G
1	A	265	A
1	A	282	A
1	A	290	U
1	A	301	G
1	A	362	A
1	A	411	G
1	A	547	A
1	A	555	G

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Mol	Chain	Res	Type
1	A	645	C
1	A	652	U
1	A	653	U
1	A	710	U
1	A	747	5MC
1	A	764	A
1	A	775	G
1	A	784	G
1	A	859	G
1	A	872	U
1	A	884	U
1	A	899	A
1	A	984	A
1	A	1020	A
1	A	1022	G
1	A	1046	A
1	A	1050	A
1	A	1069	A
1	A	1070	A
1	A	1089	A
1	A	1124	G
1	A	1130	U
1	A	1140	C
1	A	1190	G
1	A	1211	U
1	A	1240	U
1	A	1399	C
1	A	1419	A
1	A	1420	A
1	A	1432	G
1	A	1451	C
1	A	1452	G
1	A	1458	U
1	A	1475	G
1	A	1481	U
1	A	1490	A
1	A	1507	C
1	A	1508	A
1	A	1536	C
1	A	1538	G
1	A	1555	G
1	A	1607	C

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Mol	Chain	Res	Type
1	A	1608	A
1	A	1730	U
1	A	1818	U
1	A	1857	G
1	A	1875	G
1	A	1884	G
1	A	1939	5MU
1	A	1940	U
1	A	1964	G
1	A	1976	U
1	A	2099	U
1	A	2192	U
1	A	2296	U
1	A	2326	C
1	A	2391	G
1	A	2401	U
1	A	2407	A
1	A	2430	A
1	A	2517	C
1	A	2529	G
1	A	2566	A
1	A	2645	G
1	A	2712	C
1	A	2790	U
1	A	2808	G
1	A	2820	A
1	A	2849	U
1	A	2873	A
1	A	2893	A
1	A	2900	A
1	A	2902	C
2	B	4	C
2	B	34	A
2	B	41	G
2	B	44	G
2	B	46	A
2	B	56	G
2	B	89	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

52 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	7MG	y	46	57	23,26,27	1.43	4 (17%)	27,39,42	2.47	7 (25%)
1	2MG	A	1835	1	23,26,27	1.28	3 (13%)	33,38,41	2.18	7 (21%)
1	PSU	A	1917	1	18,21,22	1.41	2 (11%)	21,30,33	2.09	4 (19%)
1	PSU	A	2605	60,1	18,21,22	1.42	2 (11%)	21,30,33	2.21	4 (19%)
1	5MC	A	1962	1	19,22,23	1.49	2 (10%)	26,32,35	1.24	3 (11%)
1	PSU	A	2457	1	18,21,22	1.55	3 (16%)	21,30,33	2.00	5 (23%)
57	PSU	y	55	57	18,21,22	1.40	2 (11%)	21,30,33	2.05	5 (23%)
34	2MG	a	1516	34	23,26,27	1.27	5 (21%)	33,38,41	2.42	12 (36%)
34	4OC	a	1402	60,34	20,23,24	0.81	0	25,32,35	1.34	5 (20%)
1	PSU	A	955	1	18,21,22	1.41	3 (16%)	21,30,33	2.10	4 (19%)
1	2MG	A	2445	1	23,26,27	1.32	5 (21%)	33,38,41	2.29	8 (24%)
34	5MC	a	1407	34	19,22,23	1.68	2 (10%)	26,32,35	1.31	4 (15%)
57	PSU	y	39	57	18,21,22	1.45	2 (11%)	21,30,33	2.01	4 (19%)
34	7MG	a	527	34	23,26,27	1.45	4 (17%)	27,39,42	2.48	7 (25%)
55	PSU	w	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.06	5 (23%)
1	2MA	A	2503	60,1	22,25,26	1.51	5 (22%)	32,37,40	2.25	9 (28%)
57	PSU	y	32	57	18,21,22	1.36	2 (11%)	21,30,33	2.05	5 (23%)
34	2MG	a	1207	60,34	23,26,27	1.24	3 (13%)	33,38,41	3.00	10 (30%)
1	PSU	A	2580	1	18,21,22	1.50	3 (16%)	21,30,33	2.07	5 (23%)
57	4SU	y	8	57	18,21,22	1.81	5 (27%)	25,30,33	2.37	7 (28%)
1	OMG	A	2251	60,1,55	23,26,27	1.27	3 (13%)	32,38,41	1.94	7 (21%)
34	PSU	a	516	34	18,21,22	1.44	2 (11%)	21,30,33	2.08	5 (23%)
57	5MU	y	54	57	19,22,23	1.41	4 (21%)	27,32,35	2.12	8 (29%)
34	5MC	a	967	34	19,22,23	1.84	2 (10%)	26,32,35	1.26	3 (11%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.39	4 (21%)
1	5MC	A	747	1	19,22,23	1.84	3 (15%)	26,32,35	1.66	6 (23%)
1	OMU	A	2552	60,1	19,22,23	1.39	2 (10%)	25,31,34	2.25	8 (32%)
1	3TD	A	1915	60,1	19,22,23	7.04	13 (68%)	23,32,35	2.05	4 (17%)
55	4SU	v	7	55	18,21,22	1.75	4 (22%)	25,30,33	2.42	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	6MZ	A	1618	1	22,25,26	1.54	4 (18%)	29,36,39	2.29	10 (34%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.08	11 (40%)
1	5MU	A	1939	1	19,22,23	1.38	5 (26%)	27,32,35	2.04	8 (29%)
34	UR3	a	1498	34	19,22,23	1.09	2 (10%)	26,32,35	1.99	5 (19%)
1	PSU	A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
34	MA6	a	1519	34	23,26,27	1.70	6 (26%)	33,38,41	2.34	12 (36%)
1	PSU	A	746	60,1	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
1	6MZ	A	2030	1	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
1	PSU	A	2504	1	18,21,22	1.39	2 (11%)	21,30,33	1.94	4 (19%)
1	PSU	A	2604	1	18,21,22	1.42	3 (16%)	21,30,33	1.99	4 (19%)
1	OMC	A	2498	60,1	19,22,23	0.88	1 (5%)	25,31,34	1.23	2 (8%)
57	H2U	y	20	57	18,21,22	0.85	1 (5%)	19,30,33	1.48	4 (21%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.58	2 (10%)
55	4SU	w	8	55	18,21,22	1.81	5 (27%)	25,30,33	2.22	5 (20%)
55	H2U	v	20	55	18,21,22	0.91	1 (5%)	19,30,33	1.63	4 (21%)
57	MIA	y	37	57	28,31,32	2.44	7 (25%)	38,44,47	2.92	15 (39%)
55	PSU	v	55	60,55	18,21,22	1.38	3 (16%)	21,30,33	1.98	5 (23%)
1	1MG	A	745	1	23,26,27	1.29	3 (13%)	33,39,42	1.97	7 (21%)
1	H2U	A	2449	1	18,21,22	1.03	2 (11%)	19,30,33	1.49	3 (15%)
55	5MU	v	54	55	19,22,23	1.49	5 (26%)	27,32,35	1.91	8 (29%)
1	7MG	A	2069	60,1	23,26,27	1.49	4 (17%)	27,39,42	2.54	10 (37%)
34	2MG	a	966	34	23,26,27	1.28	3 (13%)	33,38,41	2.65	10 (30%)
34	MA6	a	1518	34	23,26,27	1.83	6 (26%)	33,38,41	2.19	10 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2605	60,1	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	1/7/25/26	0/2/2/2
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
34	4OC	a	1402	60,34	-	2/9/29/30	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/9/27/28	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
57	PSU	y	39	57	-	2/7/25/26	0/2/2/2
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	2MA	A	2503	60,1	-	0/7/25/26	0/3/3/3
57	PSU	y	32	57	-	1/7/25/26	0/2/2/2
34	2MG	a	1207	60,34	-	0/9/27/28	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
1	OMG	A	2251	60,1,55	-	0/9/27/28	0/3/3/3
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	60,1	-	2/9/27/28	0/2/2/2
1	3TD	A	1915	60,1	-	3/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	6MZ	A	1618	1	-	3/9/27/28	0/3/3/3
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	1/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	3/11/29/30	0/3/3/3
1	PSU	A	746	60,1	-	4/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	3/9/27/28	0/3/3/3
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	2/7/25/26	0/2/2/2
1	OMC	A	2498	60,1	-	0/9/27/28	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
57	MIA	y	37	57	-	5/15/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	v	55	60,55	-	2/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	7MG	A	2069	60,1	-	2/7/37/38	0/3/3/3
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.11	1.66	1.43
1	A	1915	3TD	C6-C5	16.03	1.53	1.35
1	A	1915	3TD	C2'-C1'	-14.45	1.34	1.53
1	A	1915	3TD	C2-N1	8.02	1.47	1.37
57	y	37	MIA	C13-C14	7.18	1.53	1.32
1	A	747	5MC	C5-C4	6.87	1.49	1.44
57	y	37	MIA	C2-S10	-6.66	1.70	1.75
34	a	967	5MC	C5-C4	6.63	1.49	1.44
1	A	1915	3TD	C2-N3	6.41	1.52	1.38
1	A	1915	3TD	O4'-C4'	-6.03	1.31	1.45
34	a	1407	5MC	C5-C4	5.99	1.48	1.44
34	a	1518	MA6	C5-C4	5.48	1.48	1.39
1	A	1962	5MC	C5-C4	5.27	1.48	1.44
1	A	1915	3TD	C6-N1	4.99	1.44	1.36
57	y	37	MIA	C5-C4	4.97	1.47	1.39
55	w	8	4SU	C4-S4	-4.91	1.60	1.68
57	y	8	4SU	C4-S4	-4.85	1.60	1.68
34	a	1519	MA6	C5-C4	4.78	1.47	1.39
1	A	1618	6MZ	C5-C4	4.76	1.47	1.39
55	v	7	4SU	C4-S4	-4.76	1.60	1.68
1	A	2030	6MZ	C5-C4	4.74	1.47	1.39
1	A	2069	7MG	C4-N9	-4.57	1.32	1.37
34	a	516	PSU	C6-C5	4.48	1.40	1.35
57	y	39	PSU	C6-C5	4.43	1.40	1.35
57	y	55	PSU	C6-C5	4.35	1.40	1.35
1	A	2503	2MA	C5-C4	4.33	1.46	1.39
1	A	1911	PSU	C6-C5	4.28	1.40	1.35
1	A	2457	PSU	C6-C5	4.25	1.40	1.35
55	v	55	PSU	C6-C5	4.24	1.40	1.35
1	A	2580	PSU	C6-C5	4.18	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1917	PSU	C6-C5	4.18	1.39	1.35
1	A	2605	PSU	C6-C5	4.13	1.39	1.35
57	y	32	PSU	C6-C5	4.11	1.39	1.35
55	w	55	PSU	C6-C5	4.10	1.39	1.35
1	A	2504	PSU	C6-C5	4.00	1.39	1.35
1	A	746	PSU	C6-C5	3.73	1.39	1.35
1	A	955	PSU	C6-C5	3.70	1.39	1.35
34	a	527	7MG	C4-N9	-3.68	1.33	1.37
1	A	2604	PSU	C6-C5	3.64	1.39	1.35
57	y	46	7MG	C5-C4	3.50	1.48	1.37
34	a	967	5MC	C6-C5	3.41	1.40	1.34
34	a	527	7MG	C5-C4	3.36	1.48	1.37
55	v	54	5MU	C6-C5	3.32	1.40	1.34
57	y	46	7MG	C4-N9	-3.31	1.33	1.37
57	y	37	MIA	C5-C6	3.26	1.49	1.41
1	A	2552	OMU	C2-N1	3.24	1.43	1.38
34	a	1518	MA6	C5-C6	3.23	1.49	1.41
1	A	2251	OMG	C5-C4	3.18	1.47	1.38
34	a	966	2MG	C5-C4	3.16	1.47	1.38
55	w	54	5MU	C6-C5	3.15	1.39	1.34
34	a	1407	5MC	C6-C5	3.10	1.39	1.34
55	w	54	5MU	C2-N1	3.08	1.43	1.38
34	a	1207	2MG	C5-C4	3.03	1.47	1.38
57	y	54	5MU	C2-N1	3.03	1.43	1.38
34	a	1519	MA6	C5-N7	-3.03	1.33	1.39
55	w	8	4SU	C2-N1	3.02	1.43	1.38
1	A	2069	7MG	C5-C4	3.01	1.46	1.37
34	a	1519	MA6	C5-C6	3.00	1.49	1.41
34	a	1516	2MG	C5-C4	2.98	1.46	1.38
1	A	745	1MG	C2-N1	2.97	1.42	1.37
1	A	1835	2MG	C5-C4	2.95	1.46	1.38
57	y	8	4SU	C2-N1	2.94	1.43	1.38
1	A	1915	3TD	O2'-C2'	2.93	1.50	1.43
1	A	2251	OMG	C5-N7	-2.92	1.33	1.39
1	A	1915	3TD	O2-C2	-2.91	1.17	1.23
1	A	2552	OMU	C4-N3	-2.91	1.33	1.38
57	y	8	4SU	C4-N3	-2.84	1.34	1.37
55	w	8	4SU	C4-N3	-2.83	1.34	1.37
1	A	1618	6MZ	C5-C6	2.82	1.48	1.41
1	A	2030	6MZ	C5-C6	2.82	1.48	1.41
1	A	1915	3TD	C10-N3	-2.81	1.42	1.47
1	A	745	1MG	C5-C4	2.78	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	7	4SU	C2-N1	2.76	1.42	1.38
1	A	2445	2MG	C5-C4	2.75	1.46	1.38
57	y	54	5MU	C6-C5	2.73	1.39	1.34
55	w	54	5MU	C4-C5	2.73	1.49	1.44
1	A	2580	PSU	C4-N3	-2.73	1.33	1.38
55	v	7	4SU	C4-N3	-2.72	1.34	1.37
34	a	1518	MA6	C5-N7	-2.72	1.34	1.39
1	A	2604	PSU	C4-N3	-2.71	1.33	1.38
1	A	746	PSU	C4-N3	-2.70	1.33	1.38
1	A	2504	PSU	C4-N3	-2.68	1.33	1.38
34	a	1518	MA6	C4-N9	-2.65	1.32	1.37
1	A	747	5MC	C6-C5	2.65	1.38	1.34
1	A	1915	3TD	C4-N3	2.62	1.45	1.40
55	v	54	5MU	C4-N3	-2.62	1.34	1.38
1	A	2503	2MA	C5-N7	-2.58	1.34	1.39
1	A	745	1MG	C5-N7	-2.58	1.33	1.39
55	v	54	5MU	C2-N1	2.57	1.42	1.38
1	A	2605	PSU	C4-N3	-2.56	1.34	1.38
1	A	2457	PSU	C4-N3	-2.55	1.34	1.38
1	A	1915	3TD	O3'-C3'	-2.55	1.36	1.43
57	y	8	4SU	C5-C4	-2.54	1.39	1.42
1	A	2580	PSU	C2-N3	-2.53	1.33	1.37
1	A	955	PSU	C4-N3	-2.50	1.34	1.38
1	A	2445	2MG	C6-N1	-2.49	1.34	1.38
55	v	54	5MU	C4-C5	2.49	1.48	1.44
1	A	2445	2MG	C5-N7	-2.48	1.34	1.39
34	a	966	2MG	C2-N3	2.47	1.36	1.32
1	A	1939	5MU	C6-C5	2.47	1.38	1.34
1	A	2449	H2U	C2-N3	-2.46	1.33	1.38
1	A	2457	PSU	C2-N3	-2.43	1.33	1.37
55	v	7	4SU	C5-C4	-2.42	1.39	1.42
57	y	54	5MU	C4-C5	2.41	1.48	1.44
1	A	1835	2MG	C5-N7	-2.40	1.34	1.39
1	A	1915	3TD	C3'-C4'	2.40	1.59	1.53
1	A	2449	H2U	C4-N3	-2.40	1.33	1.37
57	y	37	MIA	C8-N7	2.39	1.36	1.31
1	A	1939	5MU	C6-N1	-2.39	1.33	1.38
57	y	37	MIA	C5-N7	-2.39	1.34	1.39
1	A	1835	2MG	C6-N1	-2.39	1.34	1.38
1	A	1618	6MZ	C8-N7	2.39	1.36	1.31
1	A	2030	6MZ	C8-N7	2.38	1.36	1.31
1	A	1939	5MU	C4-N3	-2.38	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1962	5MC	C6-C5	2.37	1.38	1.34
55	w	8	4SU	C5-C4	-2.37	1.39	1.42
1	A	2503	2MA	C4-N9	-2.35	1.32	1.37
34	a	966	2MG	C5-N7	-2.33	1.34	1.39
1	A	2503	2MA	C8-N7	2.33	1.36	1.31
1	A	2503	2MA	C5-C6	2.32	1.47	1.41
34	a	1519	MA6	C4-N9	-2.32	1.32	1.37
1	A	747	5MC	C6-N1	-2.28	1.34	1.38
57	y	54	5MU	C4-N3	-2.28	1.34	1.38
34	a	516	PSU	C4-N3	-2.27	1.34	1.38
1	A	1917	PSU	C4-N3	-2.26	1.34	1.38
1	A	1618	6MZ	C5-N7	-2.25	1.35	1.39
55	w	54	5MU	C4-N3	-2.24	1.34	1.38
57	y	32	PSU	C4-N3	-2.24	1.34	1.38
1	A	2251	OMG	C6-N1	-2.24	1.34	1.38
1	A	1911	PSU	C4-N3	-2.23	1.34	1.38
1	A	1939	5MU	C4-C5	2.23	1.48	1.44
57	y	55	PSU	C4-N3	-2.22	1.34	1.38
34	a	1518	MA6	C6-N6	2.22	1.42	1.36
55	v	55	PSU	C4-N3	-2.21	1.34	1.38
1	A	2030	6MZ	C5-N7	-2.19	1.35	1.39
34	a	1516	2MG	C2-N3	2.19	1.36	1.32
1	A	746	PSU	C2-N3	-2.18	1.33	1.37
34	a	1519	MA6	C6-N6	2.18	1.42	1.36
55	w	55	PSU	C4-N3	-2.17	1.34	1.38
57	y	37	MIA	C2-N1	2.16	1.37	1.34
1	A	2069	7MG	C5-N7	-2.16	1.32	1.35
1	A	2069	7MG	C6-N1	-2.16	1.34	1.38
34	a	1516	2MG	C5-N7	-2.15	1.34	1.39
34	a	1516	2MG	C4-N9	-2.14	1.32	1.38
34	a	1498	UR3	C2-N1	2.13	1.41	1.38
34	a	1516	2MG	C6-N1	-2.13	1.34	1.38
57	y	20	H2U	C2-N3	-2.13	1.34	1.38
57	y	16	H2U	C2-N3	-2.12	1.34	1.38
57	y	46	7MG	C5-C6	2.12	1.48	1.43
34	a	1498	UR3	C5-C4	-2.11	1.38	1.43
1	A	2604	PSU	C2-N3	-2.10	1.34	1.37
55	v	54	5MU	C2-N3	-2.10	1.34	1.38
34	a	527	7MG	C8-N9	2.09	1.47	1.45
57	y	39	PSU	C4-N3	-2.09	1.34	1.38
34	a	1207	2MG	C4-N9	-2.09	1.32	1.38
57	y	46	7MG	C8-N9	2.09	1.47	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1939	5MU	C2-N1	2.08	1.41	1.38
1	A	2445	2MG	C2-N3	2.08	1.35	1.32
55	v	20	H2U	C2-N3	-2.07	1.34	1.38
55	w	8	4SU	C6-C5	2.07	1.39	1.35
1	A	2445	2MG	C4-N9	-2.07	1.32	1.38
34	a	1518	MA6	C8-N7	2.06	1.35	1.31
1	A	955	PSU	C2-N3	-2.06	1.34	1.37
1	A	2498	OMC	C5-C4	-2.04	1.38	1.42
34	a	1519	MA6	C8-N7	2.04	1.35	1.31
55	v	55	PSU	C4-C5	2.03	1.50	1.44
34	a	1207	2MG	C5-N7	-2.02	1.35	1.39
34	a	527	7MG	C6-N1	-2.01	1.35	1.38
55	w	20	H2U	C2-N3	-2.01	1.34	1.38
57	y	8	4SU	C6-C5	2.00	1.39	1.35

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1207	2MG	N1-C2-N2	8.86	125.60	116.56
57	y	37	MIA	C5-C4-N3	-8.39	118.34	127.18
34	a	966	2MG	C2-N3-C4	8.31	122.39	112.00
57	y	37	MIA	C12-C13-C14	-8.22	112.26	127.01
34	a	1207	2MG	C2-N3-C4	8.15	122.19	112.00
57	y	46	7MG	N9-C4-N3	8.06	137.26	125.46
34	a	527	7MG	N9-C4-N3	7.90	137.04	125.46
34	a	1516	2MG	C2-N3-C4	7.62	121.54	112.00
1	A	2445	2MG	C2-N3-C4	7.61	121.51	112.00
1	A	1835	2MG	C2-N3-C4	7.59	121.49	112.00
1	A	2069	7MG	N9-C4-N3	7.34	136.21	125.46
1	A	2503	2MA	C5-C4-N3	-7.23	119.57	127.18
55	v	7	4SU	C4-N3-C2	-6.90	120.70	127.31
34	a	1207	2MG	N2-C2-N3	-6.67	112.02	120.51
34	a	1498	UR3	C4-N3-C2	-6.66	119.22	124.58
1	A	2605	PSU	N1-C2-N3	6.54	122.07	115.17
34	a	966	2MG	C5-C4-N3	-6.44	118.14	128.39
57	y	8	4SU	C4-N3-C2	-6.38	121.20	127.31
1	A	2580	PSU	N1-C2-N3	6.30	121.82	115.17
1	A	2457	PSU	N1-C2-N3	6.21	121.72	115.17
1	A	2504	PSU	N1-C2-N3	6.20	121.71	115.17
1	A	1915	3TD	N1-C2-N3	6.15	120.60	116.13
1	A	2251	OMG	C5-C4-N3	-6.14	118.62	128.39
55	w	55	PSU	N1-C2-N3	6.13	121.64	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1911	PSU	N1-C2-N3	6.13	121.64	115.17
1	A	1917	PSU	N1-C2-N3	6.13	121.63	115.17
57	y	32	PSU	N1-C2-N3	6.12	121.62	115.17
55	w	8	4SU	C4-N3-C2	-6.10	121.47	127.31
1	A	2503	2MA	N3-C4-N9	6.09	134.72	126.99
1	A	2445	2MG	C5-C4-N3	-6.08	118.71	128.39
34	a	966	2MG	N1-C2-N2	6.07	122.76	116.56
1	A	746	PSU	N1-C2-N3	6.01	121.51	115.17
1	A	1835	2MG	C5-C4-N3	-5.98	118.87	128.39
57	y	37	MIA	N3-C4-N9	5.98	134.58	126.99
57	y	55	PSU	N1-C2-N3	5.93	121.42	115.17
1	A	955	PSU	N1-C2-N3	5.92	121.42	115.17
1	A	2604	PSU	N1-C2-N3	5.91	121.40	115.17
57	y	39	PSU	N1-C2-N3	5.90	121.39	115.17
34	a	1516	2MG	C5-C4-N3	-5.90	119.00	128.39
34	a	1207	2MG	C5-C4-N3	-5.88	119.03	128.39
1	A	2030	6MZ	C5-C4-N3	-5.86	118.65	126.72
55	v	55	PSU	N1-C2-N3	5.84	121.33	115.17
1	A	1618	6MZ	C5-C4-N3	-5.82	118.71	126.72
34	a	516	PSU	N1-C2-N3	5.70	121.18	115.17
1	A	1915	3TD	C4-N3-C2	-5.67	118.61	124.61
34	a	1519	MA6	C5-C4-N3	-5.61	118.99	126.72
55	v	7	4SU	C5-C4-N3	5.59	119.95	114.75
1	A	745	1MG	C5-C4-N3	-5.46	119.71	128.39
1	A	2552	OMU	N3-C2-N1	5.41	121.93	114.89
1	A	2552	OMU	C4-N3-C2	-5.32	120.01	126.61
57	y	8	4SU	C5-C4-N3	5.28	119.66	114.75
55	w	8	4SU	C5-C4-N3	5.25	119.63	114.75
55	v	54	5MU	N3-C2-N1	5.19	121.64	114.89
57	y	46	7MG	C5-C4-N3	-5.03	118.68	128.13
1	A	2069	7MG	C5-C4-N3	-5.01	118.73	128.13
1	A	1939	5MU	N3-C2-N1	4.96	121.34	114.89
34	a	527	7MG	C5-C4-N3	-4.95	118.83	128.13
34	a	1518	MA6	C2-N1-C6	4.92	123.84	111.83
55	w	54	5MU	N3-C2-N1	4.89	121.25	114.89
57	y	8	4SU	N3-C2-N1	4.83	121.17	114.89
1	A	1939	5MU	C4-N3-C2	-4.80	121.05	127.34
1	A	2069	7MG	C2-N3-C4	4.75	120.49	112.30
55	v	7	4SU	N3-C2-N1	4.75	121.08	114.89
1	A	2251	OMG	C2-N3-C4	4.73	120.45	112.30
34	a	1518	MA6	C5-C4-N3	-4.71	120.23	126.72
34	a	1519	MA6	C2-N1-C6	4.70	123.30	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1519	MA6	C4-C5-N7	-4.67	105.25	110.58
1	A	2251	OMG	N9-C4-N3	4.65	135.25	125.95
55	w	20	H2U	O4'-C1'-N1	4.63	115.61	109.30
1	A	2030	6MZ	N3-C4-N9	4.63	135.04	127.17
1	A	1618	6MZ	N3-C4-N9	4.62	135.03	127.17
57	y	46	7MG	C2-N3-C4	4.61	120.24	112.30
1	A	2069	7MG	N9-C8-N7	-4.60	96.87	103.37
1	A	745	1MG	C2-N3-C4	4.59	122.30	111.98
57	y	54	5MU	N3-C2-N1	4.59	120.87	114.89
1	A	2605	PSU	C4-N3-C2	-4.56	120.09	126.37
57	y	46	7MG	N9-C8-N7	-4.53	96.96	103.37
34	a	966	2MG	N9-C4-N3	4.48	134.91	125.95
55	w	8	4SU	N3-C2-N1	4.46	120.70	114.89
55	w	54	5MU	C4-N3-C2	-4.40	121.58	127.34
57	y	54	5MU	C4-N3-C2	-4.37	121.61	127.34
34	a	527	7MG	N9-C8-N7	-4.34	97.23	103.37
34	a	527	7MG	C2-N3-C4	4.34	119.77	112.30
57	y	37	MIA	C4-C5-N7	-4.30	105.66	110.58
34	a	1207	2MG	C6-C5-N7	4.28	138.07	130.29
57	y	54	5MU	C5-C4-N3	4.27	119.04	115.32
1	A	2445	2MG	N9-C4-N3	4.23	134.41	125.95
1	A	745	1MG	N9-C4-N3	4.22	134.39	125.95
55	v	7	4SU	C5-C4-S4	-4.19	119.52	124.31
55	v	54	5MU	C4-N3-C2	-4.19	121.85	127.34
57	y	39	PSU	O2-C2-N1	-4.18	118.47	122.79
1	A	1835	2MG	N9-C4-N3	4.17	134.29	125.95
1	A	955	PSU	C6-C5-C4	-4.15	115.37	118.17
1	A	2449	H2U	N3-C2-N1	4.15	120.82	116.65
1	A	746	PSU	C4-N3-C2	-4.11	120.70	126.37
1	A	955	PSU	C4-N3-C2	-4.10	120.72	126.37
55	w	54	5MU	C5-C4-N3	4.08	118.87	115.32
1	A	747	5MC	CM5-C5-C6	-4.06	117.36	122.85
57	y	8	4SU	C5-C4-S4	-4.05	119.67	124.31
1	A	1917	PSU	C4-N3-C2	-4.01	120.84	126.37
34	a	1516	2MG	C6-C5-N7	4.00	137.57	130.29
57	y	54	5MU	O4-C4-C5	-3.97	120.37	124.92
1	A	1911	PSU	C4-N3-C2	-3.97	120.90	126.37
55	v	54	5MU	C5-C4-N3	3.95	118.76	115.32
57	y	55	PSU	C4-N3-C2	-3.94	120.94	126.37
1	A	747	5MC	C5-C4-N3	-3.92	117.73	121.75
57	y	37	MIA	N6-C6-N1	3.92	123.58	118.33
55	w	55	PSU	C4-N3-C2	-3.89	121.01	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	966	2MG	N2-C2-N3	-3.88	115.56	120.51
1	A	2604	PSU	C4-N3-C2	-3.88	121.02	126.37
34	a	1518	MA6	O4'-C1'-N9	3.88	115.54	108.09
57	y	32	PSU	C4-N3-C2	-3.83	121.10	126.37
57	y	37	MIA	C16-C14-C13	-3.80	111.25	122.66
34	a	1518	MA6	N1-C2-N3	-3.80	122.83	128.58
34	a	1519	MA6	N3-C4-N9	3.80	133.62	127.17
1	A	1939	5MU	O4-C4-C5	-3.77	120.61	124.92
55	v	55	PSU	C4-N3-C2	-3.75	121.20	126.37
1	A	2030	6MZ	C2-N3-C4	3.70	120.88	111.83
1	A	1618	6MZ	C2-N3-C4	3.70	120.86	111.83
55	w	8	4SU	C5-C4-S4	-3.69	120.09	124.31
1	A	2552	OMU	C1'-N1-C2	3.68	124.19	117.59
1	A	2504	PSU	C4-N3-C2	-3.66	121.32	126.37
34	a	516	PSU	C4-N3-C2	-3.66	121.33	126.37
34	a	1516	2MG	N9-C4-N3	3.66	133.27	125.95
1	A	746	PSU	O2-C2-N1	-3.63	119.04	122.79
1	A	1939	5MU	C5-C4-N3	3.63	118.48	115.32
34	a	1498	UR3	C1'-N1-C2	3.62	122.97	117.04
34	a	1519	MA6	C10-N6-C6	-3.60	111.35	120.52
34	a	1516	2MG	N1-C2-N2	3.59	120.22	116.56
1	A	2552	OMU	C5-C4-N3	3.59	119.83	114.80
1	A	2605	PSU	O2-C2-N1	-3.57	119.11	122.79
57	y	54	5MU	C5M-C5-C4	3.56	122.58	118.78
34	a	1518	MA6	C4-C5-N7	-3.56	106.52	110.58
1	A	955	PSU	O2-C2-N1	-3.53	119.15	122.79
1	A	1911	PSU	O2-C2-N1	-3.53	119.15	122.79
57	y	37	MIA	C2-N3-C4	3.51	121.49	112.29
55	w	55	PSU	O2-C2-N1	-3.51	119.17	122.79
1	A	2580	PSU	C4-N3-C2	-3.50	121.55	126.37
34	a	1207	2MG	C4-C5-N7	-3.48	105.15	110.67
57	y	32	PSU	O2-C2-N1	-3.48	119.20	122.79
1	A	2030	6MZ	C4-C5-N7	-3.48	106.61	110.58
1	A	1618	6MZ	C4-C5-N7	-3.46	106.63	110.58
57	y	39	PSU	C4-N3-C2	-3.45	121.61	126.37
34	a	1518	MA6	C2-N3-C4	3.44	120.24	111.83
34	a	1498	UR3	C5-C4-N3	3.43	119.56	115.04
34	a	1519	MA6	C2-N3-C4	3.43	120.20	111.83
57	y	37	MIA	C15-C14-C13	-3.39	112.49	122.66
57	y	55	PSU	O2-C2-N1	-3.39	119.30	122.79
57	y	39	PSU	C6-C5-C4	-3.38	115.90	118.17
1	A	1618	6MZ	C6-C5-N7	3.38	136.11	132.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2503	2MA	N6-C6-N1	3.37	121.58	117.03
1	A	2030	6MZ	C6-C5-N7	3.37	136.10	132.43
57	y	37	MIA	C6-C5-N7	3.36	136.09	132.43
1	A	1917	PSU	C6-C5-C4	-3.35	115.91	118.17
1	A	745	1MG	N2-C2-N1	3.34	121.47	118.79
34	a	516	PSU	C3'-C2'-C1'	3.34	105.63	101.69
1	A	2457	PSU	C4-N3-C2	-3.32	121.80	126.37
55	w	54	5MU	C5M-C5-C4	3.32	122.32	118.78
55	v	55	PSU	O2-C2-N1	-3.32	119.37	122.79
1	A	1917	PSU	O2-C2-N1	-3.30	119.39	122.79
1	A	2445	2MG	C6-C5-N7	3.29	136.28	130.29
1	A	2503	2MA	C4-N9-C8	3.29	109.19	105.74
34	a	966	2MG	C6-C5-N7	3.29	136.27	130.29
34	a	1518	MA6	C9-N6-C6	-3.28	112.18	120.52
34	a	1207	2MG	N9-C4-N3	3.26	132.47	125.95
34	a	1519	MA6	N1-C2-N3	-3.25	123.67	128.58
34	a	1519	MA6	C5-N7-C8	3.23	108.53	103.45
34	a	516	PSU	C6-C5-C4	-3.22	116.00	118.17
1	A	1618	6MZ	N1-C2-N3	-3.22	123.71	128.58
1	A	1835	2MG	C6-C5-N7	3.20	136.12	130.29
1	A	1911	PSU	C6-C5-C4	-3.20	116.01	118.17
55	w	54	5MU	O4-C4-C5	-3.20	121.26	124.92
55	v	20	H2U	C3'-C2'-C1'	3.20	107.51	101.46
1	A	2030	6MZ	N1-C2-N3	-3.19	123.76	128.58
1	A	2457	PSU	O2-C2-N1	-3.15	119.54	122.79
1	A	1962	5MC	O2-C2-N3	-3.15	117.37	122.33
34	a	1516	2MG	C4-C5-N7	-3.14	105.70	110.67
57	y	20	H2U	O4'-C1'-N1	3.13	113.57	109.30
55	v	20	H2U	N3-C2-N1	3.13	119.80	116.65
34	a	967	5MC	O2-C2-N3	-3.13	117.40	122.33
34	a	1518	MA6	N3-C4-N9	3.13	132.48	127.17
1	A	2498	OMC	O2-C2-N3	-3.12	117.41	122.33
1	A	1618	6MZ	C9-N6-C6	-3.12	119.96	122.85
1	A	746	PSU	C6-C5-C4	-3.11	116.07	118.17
34	a	1407	5MC	O2-C2-N3	-3.11	117.42	122.33
57	y	37	MIA	C5-N7-C8	3.09	108.31	103.45
1	A	2030	6MZ	C9-N6-C6	-3.08	120.00	122.85
34	a	1407	5MC	C5-C4-N3	-3.06	118.61	121.75
34	a	967	5MC	C5-C4-N3	-3.06	118.62	121.75
57	y	8	4SU	C6-N1-C2	-3.06	117.28	121.00
1	A	2504	PSU	O2-C2-N1	-3.05	119.64	122.79
57	y	55	PSU	C6-C5-C4	-3.03	116.13	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2069	7MG	C5-C6-N1	2.97	116.16	110.94
1	A	2605	PSU	C6-C5-C4	-2.96	116.18	118.17
55	v	54	5MU	O4-C4-C5	-2.96	121.53	124.92
34	a	527	7MG	C5-C6-N1	2.96	116.14	110.94
1	A	2552	OMU	O4-C4-C5	-2.93	120.10	125.16
57	y	46	7MG	C5-C6-N1	2.92	116.08	110.94
55	v	20	H2U	C5-C4-N3	2.90	119.78	116.69
55	w	55	PSU	C3'-C2'-C1'	2.89	105.10	101.69
34	a	516	PSU	O2-C2-N1	-2.88	119.82	122.79
1	A	1962	5MC	C5-C4-N3	-2.87	118.81	121.75
1	A	2552	OMU	O2-C2-N3	-2.85	116.22	121.49
55	w	20	H2U	C5-C6-N1	-2.85	102.91	111.52
55	v	55	PSU	C6-C5-C4	-2.83	116.26	118.17
1	A	1939	5MU	C5-C6-N1	-2.82	120.25	123.31
1	A	2445	2MG	N1-C2-N2	2.75	119.36	116.56
1	A	2604	PSU	O2-C2-N1	-2.73	119.97	122.79
1	A	2503	2MA	C4-C5-N7	-2.73	107.47	110.58
57	y	20	H2U	C5-C4-N3	2.72	119.58	116.69
1	A	2580	PSU	C3'-C2'-C1'	2.69	104.86	101.69
57	y	37	MIA	O4'-C1'-N9	2.68	113.24	108.09
34	a	1402	4OC	C6-C5-C4	2.67	120.22	117.00
1	A	2251	OMG	O6-C6-C5	-2.67	119.50	126.53
1	A	1618	6MZ	C4-N9-C8	2.67	108.54	105.74
1	A	747	5MC	O2-C2-N3	-2.63	118.18	122.33
34	a	1518	MA6	C3'-C2'-C1'	2.63	106.44	101.46
1	A	2030	6MZ	C4-N9-C8	2.62	108.49	105.74
1	A	2604	PSU	C6-C5-C4	-2.62	116.41	118.17
55	w	8	4SU	C6-N1-C2	-2.62	117.81	121.00
1	A	2580	PSU	O2-C2-N3	-2.59	117.26	121.86
1	A	2445	2MG	C4-C5-N7	-2.59	106.57	110.67
1	A	2552	OMU	C6-N1-C2	-2.57	117.86	121.00
57	y	16	H2U	C5-C4-N3	2.57	119.42	116.69
34	a	1516	2MG	N2-C2-N3	-2.56	117.25	120.51
55	v	20	H2U	O4'-C1'-N1	2.55	112.77	109.30
1	A	1618	6MZ	C5-N7-C8	2.54	107.44	103.45
1	A	2503	2MA	C2-N1-C6	2.54	122.00	118.10
34	a	966	2MG	C4-C5-N7	-2.54	106.65	110.67
34	a	1498	UR3	C3U-N3-C2	2.54	121.75	117.33
34	a	1207	2MG	C2-N1-C6	-2.54	121.48	124.55
1	A	2030	6MZ	C5-N7-C8	2.53	107.42	103.45
1	A	2580	PSU	C6-C5-C4	-2.50	116.49	118.17
57	y	32	PSU	C6-C5-C4	-2.50	116.49	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	37	MIA	C2-N1-C6	2.50	122.28	117.54
55	v	7	4SU	C6-N1-C2	-2.49	117.96	121.00
57	y	37	MIA	C16-C14-C15	-2.49	108.86	114.59
1	A	1618	6MZ	C3'-C2'-C1'	2.48	106.16	101.46
1	A	2030	6MZ	C3'-C2'-C1'	2.48	106.15	101.46
57	y	32	PSU	C3'-C2'-C1'	2.48	104.61	101.69
57	y	16	H2U	O4'-C1'-N1	2.46	112.65	109.30
34	a	1519	MA6	C4-C5-C6	2.46	118.45	115.91
34	a	527	7MG	O4'-C1'-N9	2.45	112.63	109.30
34	a	1402	4OC	O4'-C1'-N1	2.44	113.88	108.36
1	A	1835	2MG	N1-C2-N2	2.44	119.05	116.56
34	a	966	2MG	O6-C6-C5	-2.43	120.12	126.53
1	A	2457	PSU	C6-C5-C4	-2.42	116.54	118.17
1	A	2498	OMC	O4'-C1'-N1	2.41	113.83	108.36
57	y	37	MIA	N3-C2-N1	-2.41	122.59	127.00
1	A	747	5MC	C3'-C2'-C1'	2.41	106.03	101.46
1	A	2069	7MG	O4'-C1'-N9	2.41	112.58	109.30
57	y	20	H2U	C3'-C2'-C1'	2.40	106.00	101.46
1	A	2449	H2U	C5-C4-N3	2.39	119.23	116.69
34	a	1402	4OC	C2'-C1'-N1	-2.38	109.72	114.24
55	w	55	PSU	C6-C5-C4	-2.38	116.57	118.17
1	A	747	5MC	C5-C6-N1	-2.38	120.73	123.31
1	A	1962	5MC	CM5-C5-C6	-2.37	119.64	122.85
34	a	1516	2MG	C2-N1-C6	-2.37	121.69	124.55
1	A	2069	7MG	N2-C2-N3	-2.37	115.05	119.67
34	a	967	5MC	C3'-C2'-C1'	2.36	105.93	101.46
55	v	54	5MU	C6-N1-C2	-2.35	118.96	121.30
34	a	1402	4OC	O2-C2-N3	-2.35	118.62	122.33
1	A	1939	5MU	O2-C2-N1	-2.34	119.75	122.80
1	A	2503	2MA	N9-C8-N7	-2.33	110.63	113.94
1	A	745	1MG	O6-C6-C5	-2.32	118.61	124.59
34	a	1402	4OC	C5-C4-N3	-2.32	118.97	122.60
1	A	2251	OMG	C6-C5-N7	2.32	134.50	130.29
57	y	54	5MU	C1'-N1-C2	2.31	121.74	117.59
1	A	2552	OMU	O4'-C1'-N1	2.30	113.58	108.36
1	A	2445	2MG	O6-C6-C5	-2.30	120.47	126.53
1	A	1835	2MG	O6-C6-C5	-2.30	120.47	126.53
57	y	8	4SU	O2-C2-N3	-2.29	117.26	121.49
34	a	1516	2MG	O6-C6-C5	-2.29	120.48	126.53
34	a	1407	5MC	O4'-C1'-N1	2.29	113.55	108.36
55	w	54	5MU	C5M-C5-C6	-2.29	119.75	122.85
34	a	527	7MG	O6-C6-C5	-2.29	122.01	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1835	2MG	C4-C5-N7	-2.28	107.06	110.67
1	A	1915	3TD	C3'-C2'-C1'	2.27	104.36	101.69
57	y	16	H2U	C3'-C2'-C1'	2.27	105.75	101.46
1	A	2251	OMG	O2'-C2'-C1'	2.26	113.29	108.99
57	y	54	5MU	C5M-C5-C6	-2.26	119.79	122.85
55	w	54	5MU	C3'-C2'-C1'	2.26	105.73	101.46
34	a	1519	MA6	C9-N6-C6	-2.26	114.78	120.52
1	A	2503	2MA	C5-N7-C8	2.25	106.99	103.45
55	w	54	5MU	O4'-C1'-N1	2.25	113.47	108.36
1	A	2504	PSU	C6-C5-C4	-2.25	116.65	118.17
1	A	1939	5MU	C5M-C5-C4	2.25	121.18	118.78
34	a	966	2MG	C2-N1-C6	-2.24	121.84	124.55
1	A	2445	2MG	C2-N1-C6	-2.24	121.84	124.55
1	A	745	1MG	C4-C5-N7	-2.23	107.14	110.67
57	y	8	4SU	C1'-N1-C2	2.22	121.58	117.59
1	A	745	1MG	C6-C5-N7	2.21	134.28	129.36
1	A	2069	7MG	O6-C6-C5	-2.21	122.19	127.62
34	a	966	2MG	C5-C6-N1	2.21	118.87	113.25
34	a	1519	MA6	C10-N6-C9	-2.20	109.11	116.18
1	A	2069	7MG	N2-C2-N1	2.18	121.37	116.76
34	a	1407	5MC	C5-C6-N1	-2.18	120.94	123.31
34	a	1516	2MG	C2'-C1'-N9	-2.17	107.22	113.25
55	v	54	5MU	C5-C6-N1	-2.17	120.96	123.31
57	y	46	7MG	C6-C5-C4	-2.14	118.63	122.40
1	A	2503	2MA	C6-C5-N7	2.14	136.22	132.09
1	A	747	5MC	N1-C2-N3	2.14	122.51	118.80
34	a	1207	2MG	O6-C6-C5	-2.13	120.91	126.53
57	y	46	7MG	O6-C6-C5	-2.13	122.39	127.62
55	v	54	5MU	O4'-C1'-N1	2.11	113.13	108.36
34	a	1516	2MG	O4'-C1'-N9	2.10	113.12	108.36
55	v	54	5MU	O2-C2-N3	-2.09	117.64	121.49
57	y	54	5MU	C6-N1-C2	-2.09	119.23	121.30
34	a	1518	MA6	C5-N7-C8	2.08	106.72	103.45
34	a	1207	2MG	C8-N7-C5	2.08	107.96	104.26
1	A	2251	OMG	C4-C5-N7	-2.08	107.38	110.67
34	a	1516	2MG	C5-C6-N1	2.07	118.52	113.25
55	w	54	5MU	C5-C6-N1	-2.06	121.07	123.31
57	y	55	PSU	C3'-C2'-C1'	2.06	104.12	101.69
1	A	1915	3TD	O4-C4-C5	-2.06	119.02	122.58
34	a	1519	MA6	N9-C8-N7	-2.06	111.02	113.94
1	A	2449	H2U	O4'-C1'-N1	2.05	112.10	109.30
57	y	16	H2U	C5-C6-N1	-2.05	105.31	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	54	5MU	O2-C2-N3	-2.05	117.71	121.49
57	y	20	H2U	C5-C6-N1	-2.05	105.33	111.52
55	v	55	PSU	C3'-C2'-C1'	2.04	104.09	101.69
1	A	2457	PSU	C3'-C2'-C1'	2.03	104.08	101.69
55	w	54	5MU	C6-N1-C2	-2.01	119.30	121.30
1	A	1939	5MU	C5M-C5-C6	-2.01	120.13	122.85
34	a	1498	UR3	O4-C4-C5	-2.01	118.66	124.35
1	A	2069	7MG	C6-C5-C4	-2.01	118.87	122.40
57	y	37	MIA	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	C2'-C1'-C5-C4
1	A	746	PSU	O4'-C1'-C5-C6
1	A	2030	6MZ	C4'-C5'-O5'-P
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2069	7MG	O4'-C4'-C5'-O5'
1	A	2445	2MG	O4'-C4'-C5'-O5'
1	A	2552	OMU	O4'-C1'-N1-C2
1	A	2552	OMU	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C6
34	a	1498	UR3	O4'-C1'-N1-C2
34	a	1518	MA6	C5-C6-N6-C9
34	a	1519	MA6	C5-C6-N6-C10
55	v	20	H2U	O4'-C1'-N1-C2
55	v	20	H2U	O4'-C1'-N1-C6
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
55	w	8	4SU	O4'-C4'-C5'-O5'
57	y	20	H2U	O4'-C1'-N1-C2
57	y	20	H2U	O4'-C1'-N1-C6
57	y	37	MIA	O4'-C4'-C5'-O5'
57	y	37	MIA	C12-C13-C14-C15
57	y	37	MIA	C12-C13-C14-C16
1	A	1962	5MC	O4'-C4'-C5'-O5'
1	A	2069	7MG	C3'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	2504	PSU	O4'-C4'-C5'-O5'
34	a	1402	4OC	O4'-C4'-C5'-O5'
55	w	8	4SU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
34	a	1518	MA6	O4'-C1'-N9-C8
1	A	1917	PSU	O4'-C4'-C5'-O5'
1	A	2030	6MZ	O4'-C4'-C5'-O5'
34	a	1518	MA6	O4'-C1'-N9-C4
34	a	1518	MA6	N1-C6-N6-C9
34	a	1519	MA6	N1-C6-N6-C10
55	w	8	4SU	C2'-C1'-N1-C6
57	y	37	MIA	C3'-C4'-C5'-O5'
1	A	1915	3TD	C3'-C4'-C5'-O5'
34	a	1402	4OC	C3'-C4'-C5'-O5'
57	y	46	7MG	O4'-C4'-C5'-O5'
55	w	8	4SU	C2'-C1'-N1-C2
1	A	1962	5MC	C3'-C4'-C5'-O5'
1	A	2504	PSU	C3'-C4'-C5'-O5'
1	A	2604	PSU	O4'-C4'-C5'-O5'
57	y	16	H2U	O4'-C4'-C5'-O5'
57	y	46	7MG	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C4'-C5'-O5'
55	v	7	4SU	O4'-C4'-C5'-O5'
55	v	20	H2U	O4'-C4'-C5'-O5'
55	v	20	H2U	C4'-C5'-O5'-P
1	A	1917	PSU	C3'-C4'-C5'-O5'
57	y	16	H2U	C3'-C4'-C5'-O5'
57	y	46	7MG	C2'-C1'-N9-C8
1	A	1618	6MZ	C3'-C4'-C5'-O5'
55	v	20	H2U	C3'-C4'-C5'-O5'
34	a	527	7MG	C3'-C4'-C5'-O5'
55	w	8	4SU	O4'-C1'-N1-C6
55	w	8	4SU	O4'-C1'-N1-C2
1	A	1618	6MZ	O4'-C4'-C5'-O5'
1	A	2604	PSU	C3'-C4'-C5'-O5'
34	a	527	7MG	C4'-C5'-O5'-P
34	a	966	2MG	C3'-C4'-C5'-O5'
1	A	746	PSU	O4'-C1'-C5-C4
57	y	32	PSU	O4'-C1'-C5-C4
57	y	39	PSU	O4'-C1'-C5-C4
34	a	1519	MA6	C4'-C5'-O5'-P
1	A	2457	PSU	O4'-C4'-C5'-O5'
55	v	7	4SU	C3'-C4'-C5'-O5'
34	a	966	2MG	C4'-C5'-O5'-P
1	A	1939	5MU	O4'-C4'-C5'-O5'
55	w	20	H2U	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
57	y	46	7MG	O4'-C1'-N9-C8
55	w	55	PSU	O4'-C1'-C5-C6
57	y	39	PSU	O4'-C1'-C5-C6
34	a	966	2MG	O4'-C4'-C5'-O5'
57	y	37	MIA	N3-C2-S10-C11
1	A	746	PSU	C2'-C1'-C5-C6
1	A	1915	3TD	C2'-C1'-C5-C6
57	y	8	4SU	C2'-C1'-N1-C2
1	A	1618	6MZ	C4'-C5'-O5'-P

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2445	2MG	1	0
34	a	1207	2MG	1	0
1	A	1915	3TD	2	0
1	A	1618	6MZ	1	0
1	A	1939	5MU	1	0
34	a	1519	MA6	1	0
1	A	2030	6MZ	10	0
1	A	2504	PSU	1	0
1	A	2604	PSU	1	0
34	a	1518	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1481 ligands modelled in this entry, 1478 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	GTP	z	402	60	33,34,34	1.17	3 (9%)	50,54,54	1.74	7 (14%)
59	FME	A	3001	-	8,9,10	0.52	0	8,9,11	1.03	0
62	PHE	z	401	-	10,11,12	0.39	0	8,13,15	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	GTP	z	402	60	-	7/22/38/38	0/3/3/3
59	FME	A	3001	-	-	0/7/9/11	-
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	C5-C4	3.08	1.47	1.38
63	z	402	GTP	C6-N1	-2.68	1.33	1.38
63	z	402	GTP	C5-N7	-2.14	1.34	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GTP	C5-C4-N3	-6.33	118.31	128.39
63	z	402	GTP	C2-N3-C4	5.18	121.22	112.30
63	z	402	GTP	N9-C4-N3	4.80	135.55	125.95
63	z	402	GTP	C6-C5-N7	3.10	135.93	130.29
63	z	402	GTP	C4-C5-N7	-2.40	106.86	110.67
63	z	402	GTP	C3'-C2'-C1'	2.25	105.71	101.46
63	z	402	GTP	O6-C6-C5	-2.18	120.78	126.53

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	z	401	PHE	O-C-CA-CB
63	z	402	GTP	C5'-O5'-PA-O3A
63	z	402	GTP	C5'-O5'-PA-O1A
63	z	402	GTP	C5'-O5'-PA-O2A
63	z	402	GTP	C3'-C4'-C5'-O5'

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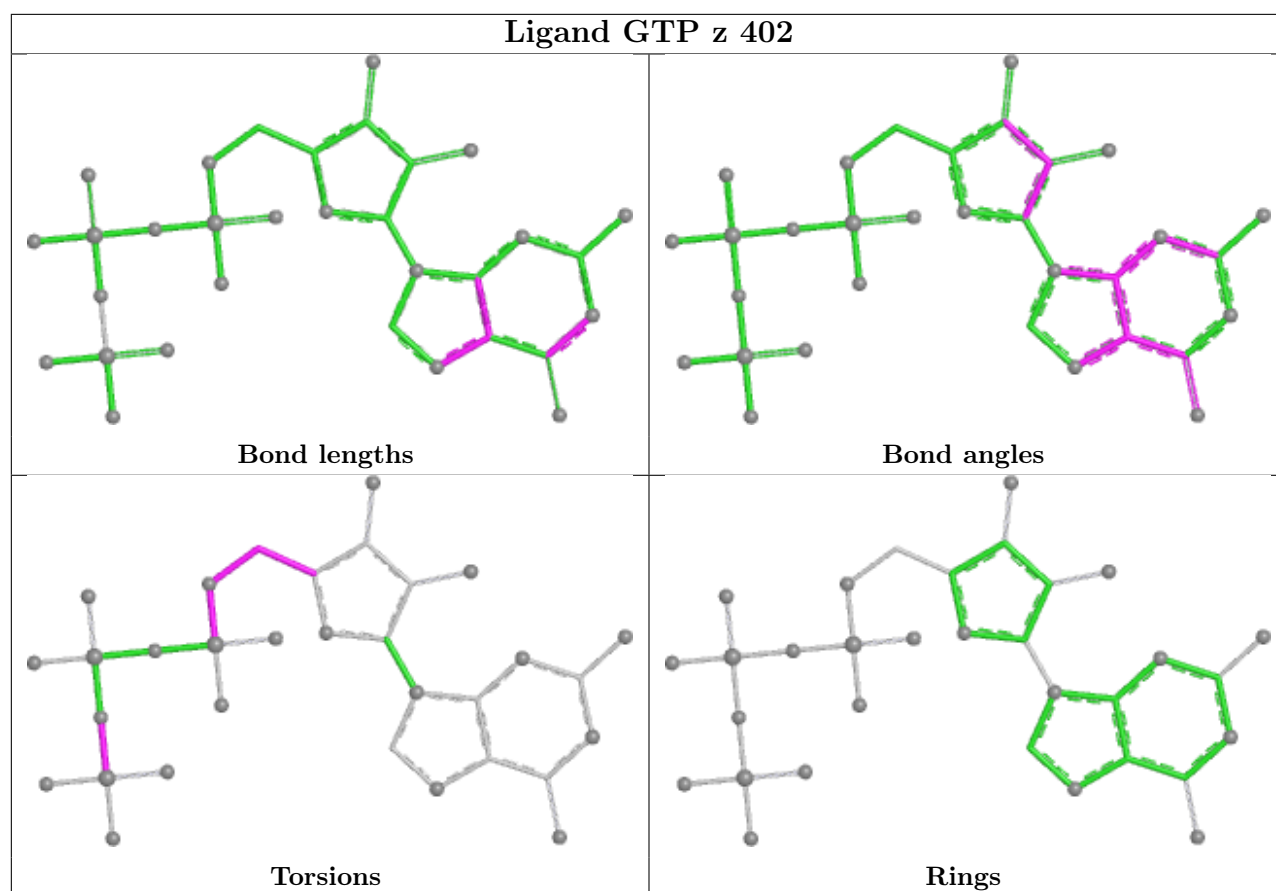
Mol	Chain	Res	Type	Atoms
63	z	402	GTP	O4'-C4'-C5'-O5'
63	z	402	GTP	PB-O3B-PG-O1G
63	z	402	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	z	402	GTP	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

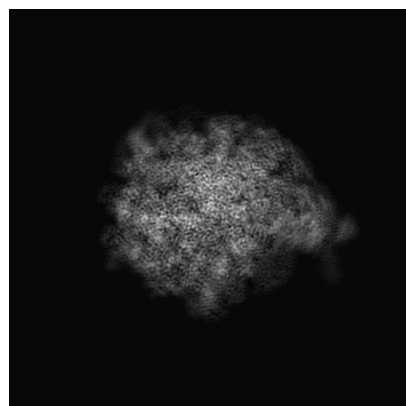
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8829. These allow visual inspection of the internal detail of the map and identification of artifacts.

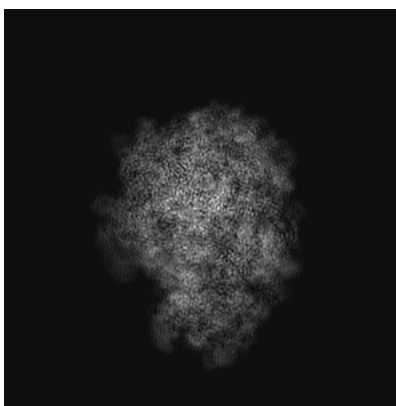
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

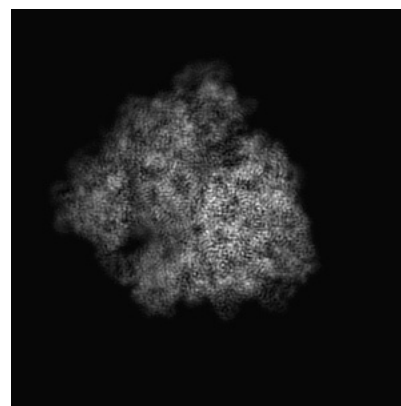
6.1.1 Primary map



X

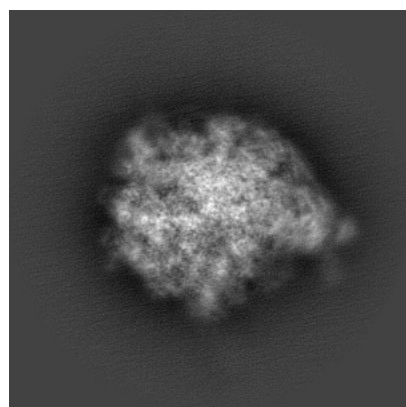


Y

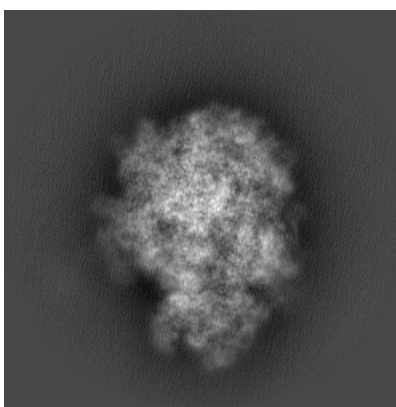


Z

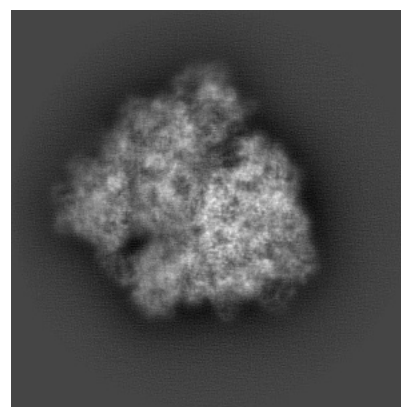
6.1.2 Raw map



X



Y

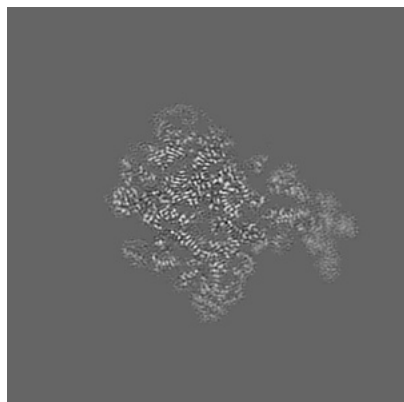


Z

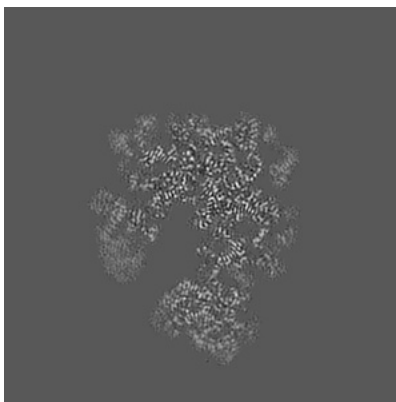
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

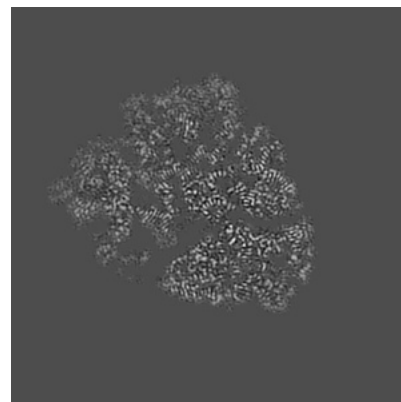
6.2.1 Primary map



X Index: 199

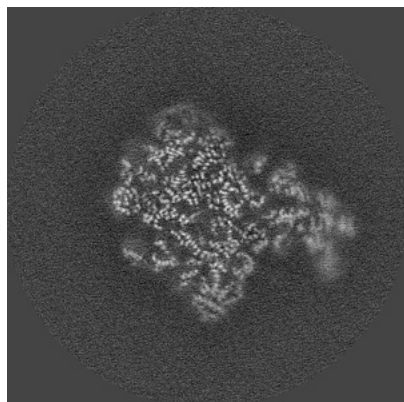


Y Index: 199

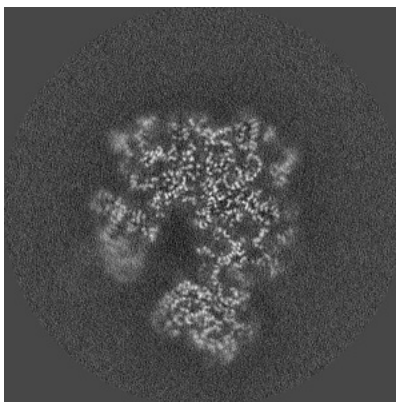


Z Index: 199

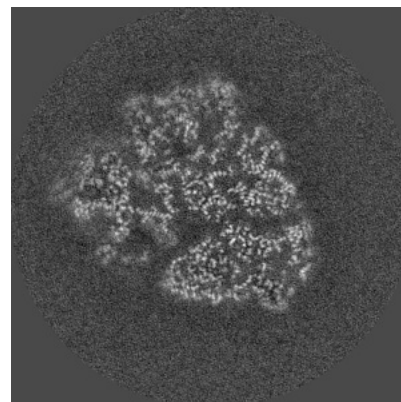
6.2.2 Raw map



X Index: 199



Y Index: 199

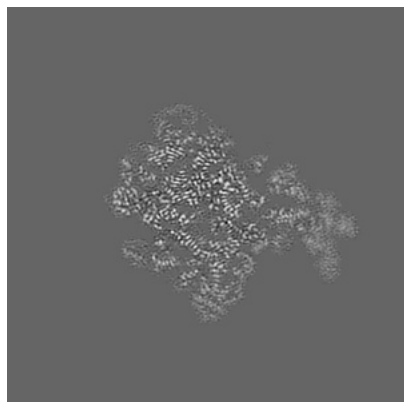


Z Index: 199

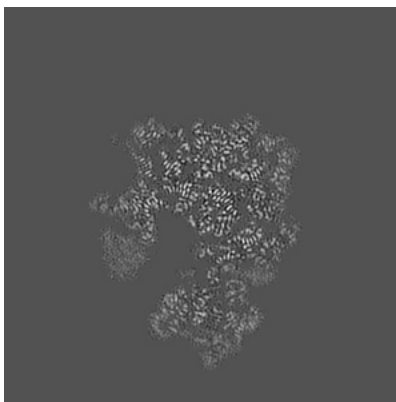
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

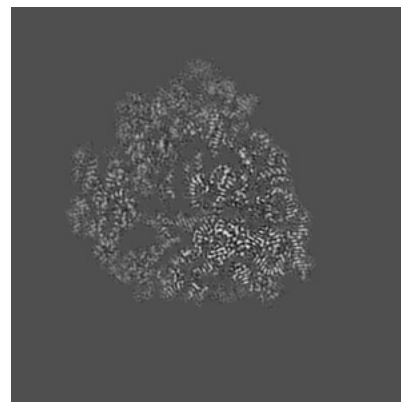
6.3.1 Primary map



X Index: 199

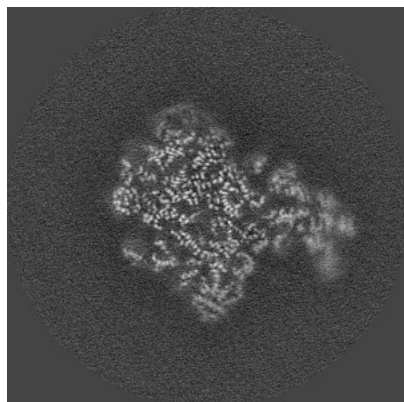


Y Index: 207

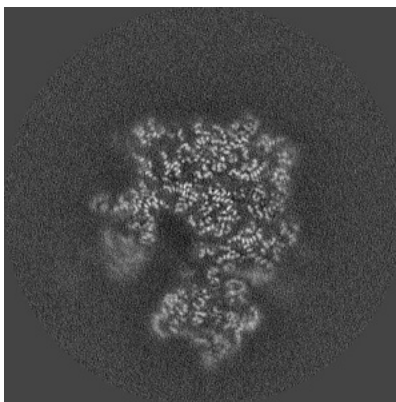


Z Index: 190

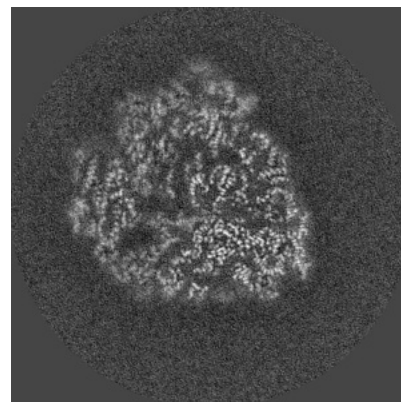
6.3.2 Raw map



X Index: 199



Y Index: 207

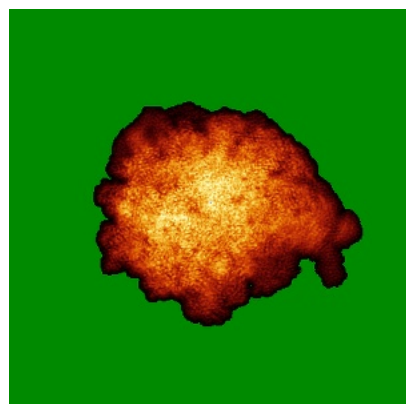


Z Index: 190

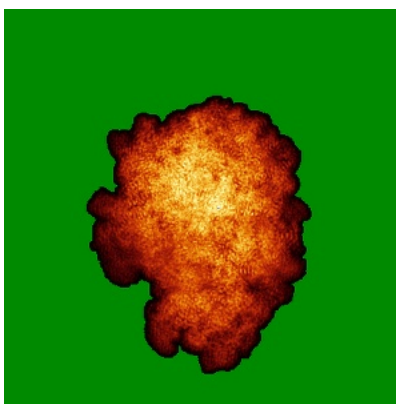
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

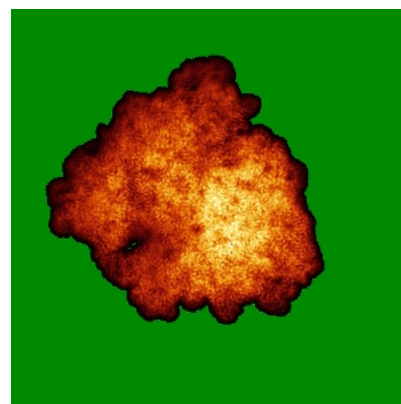
6.4.1 Primary map



X

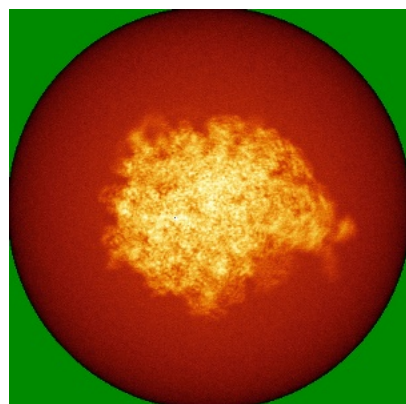


Y

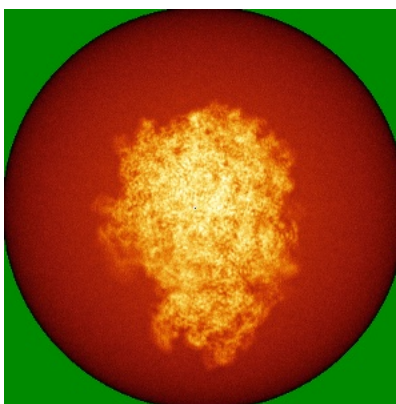


Z

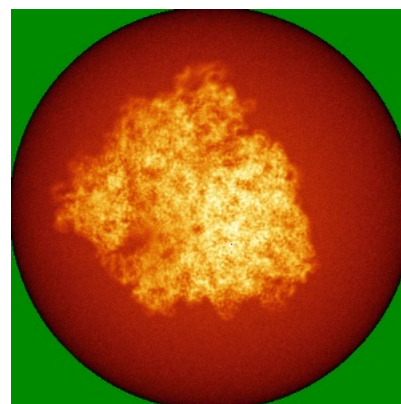
6.4.2 Raw map



X



Y

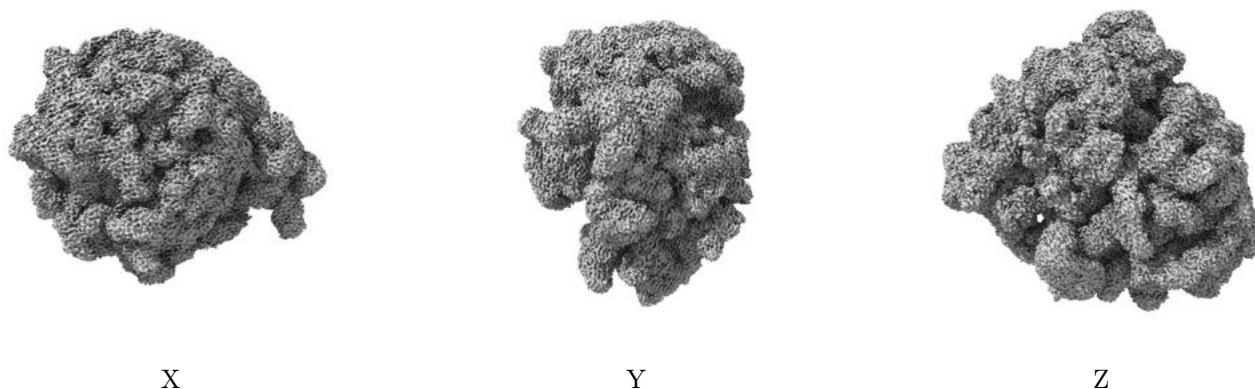


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

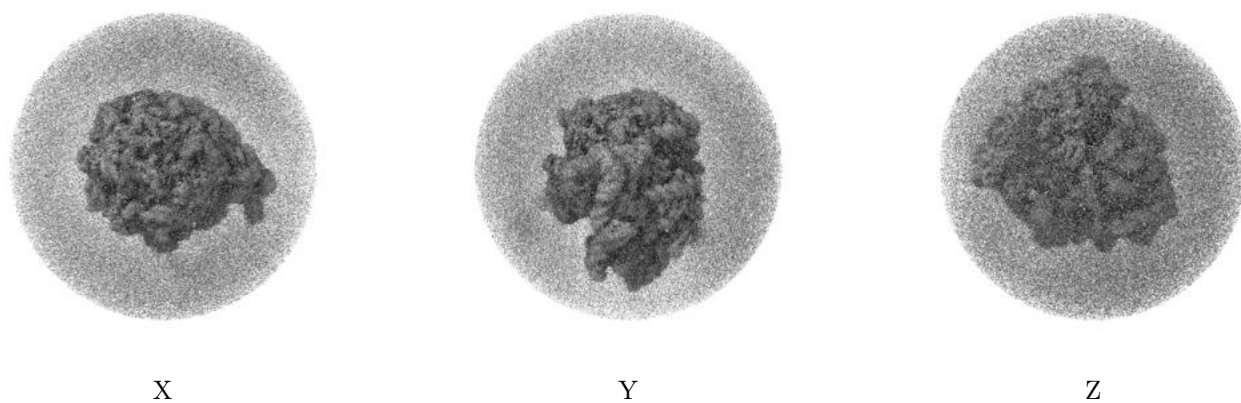
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00532. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

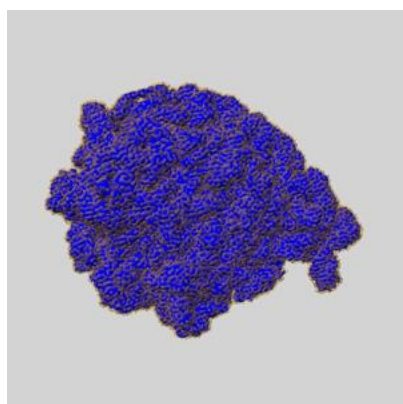
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

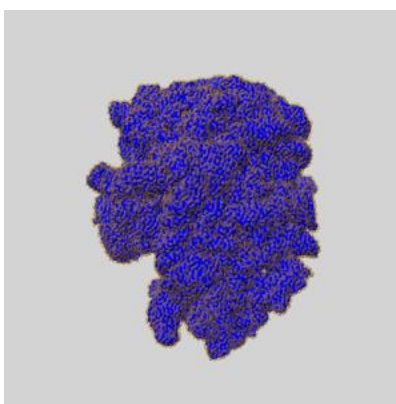
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

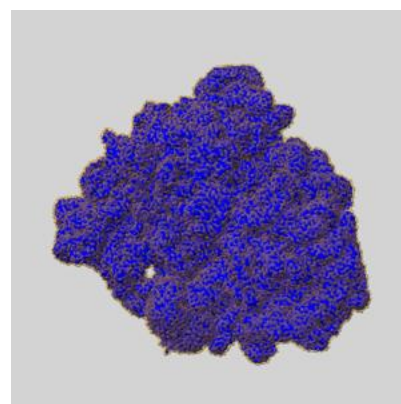
6.6.1 emd_8829_msk_1.map [i](#)



X



Y

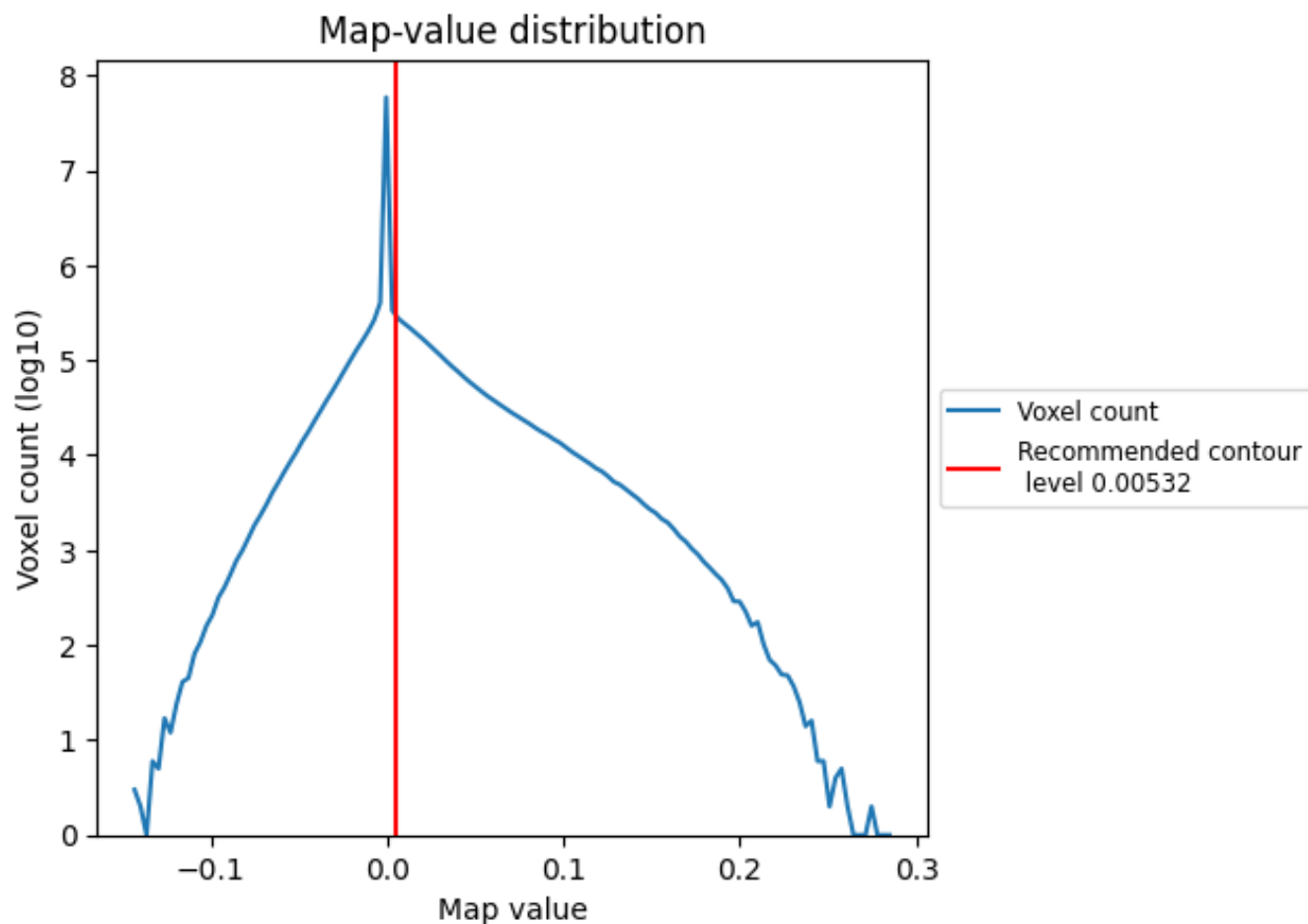


Z

7 Map analysis [i](#)

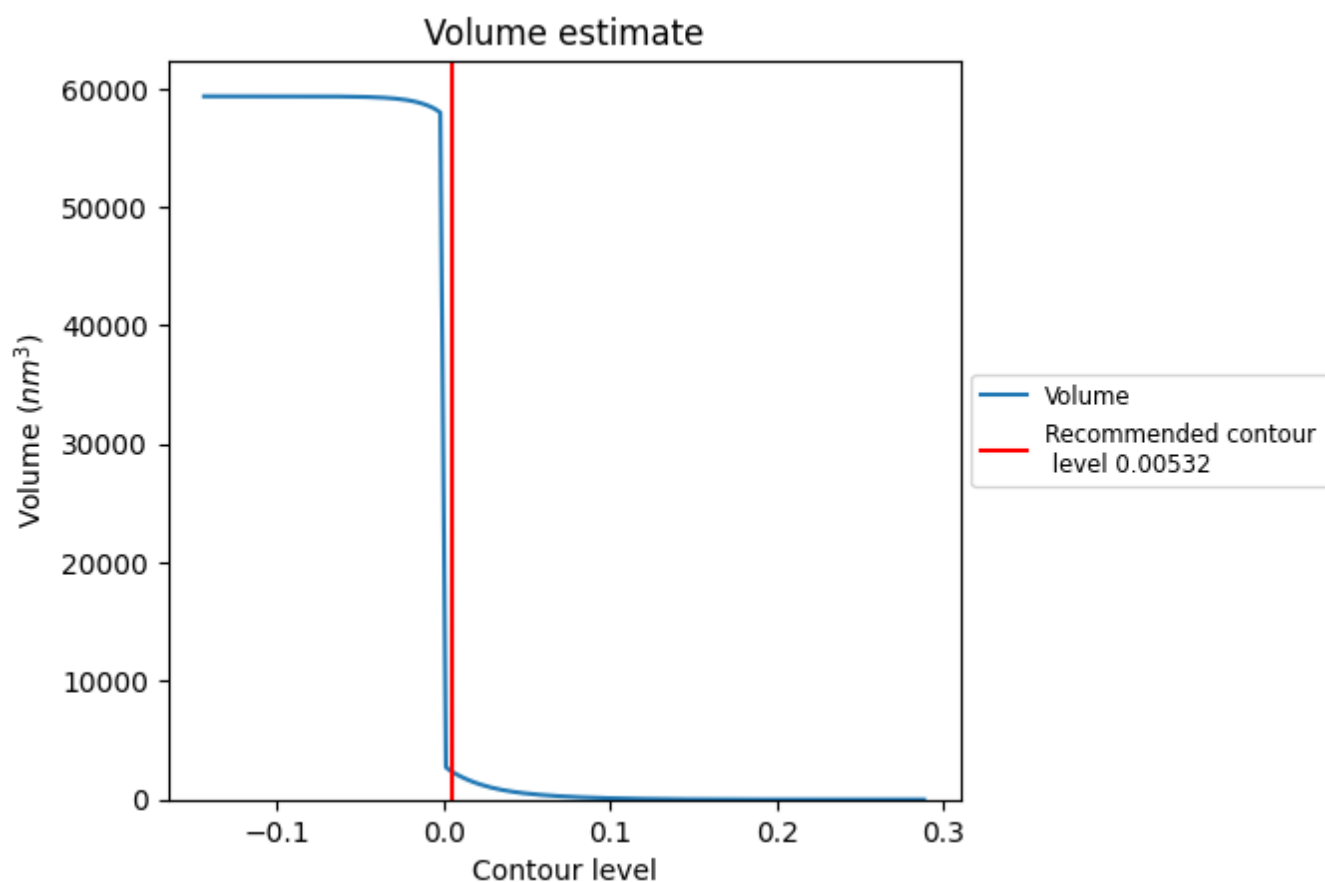
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

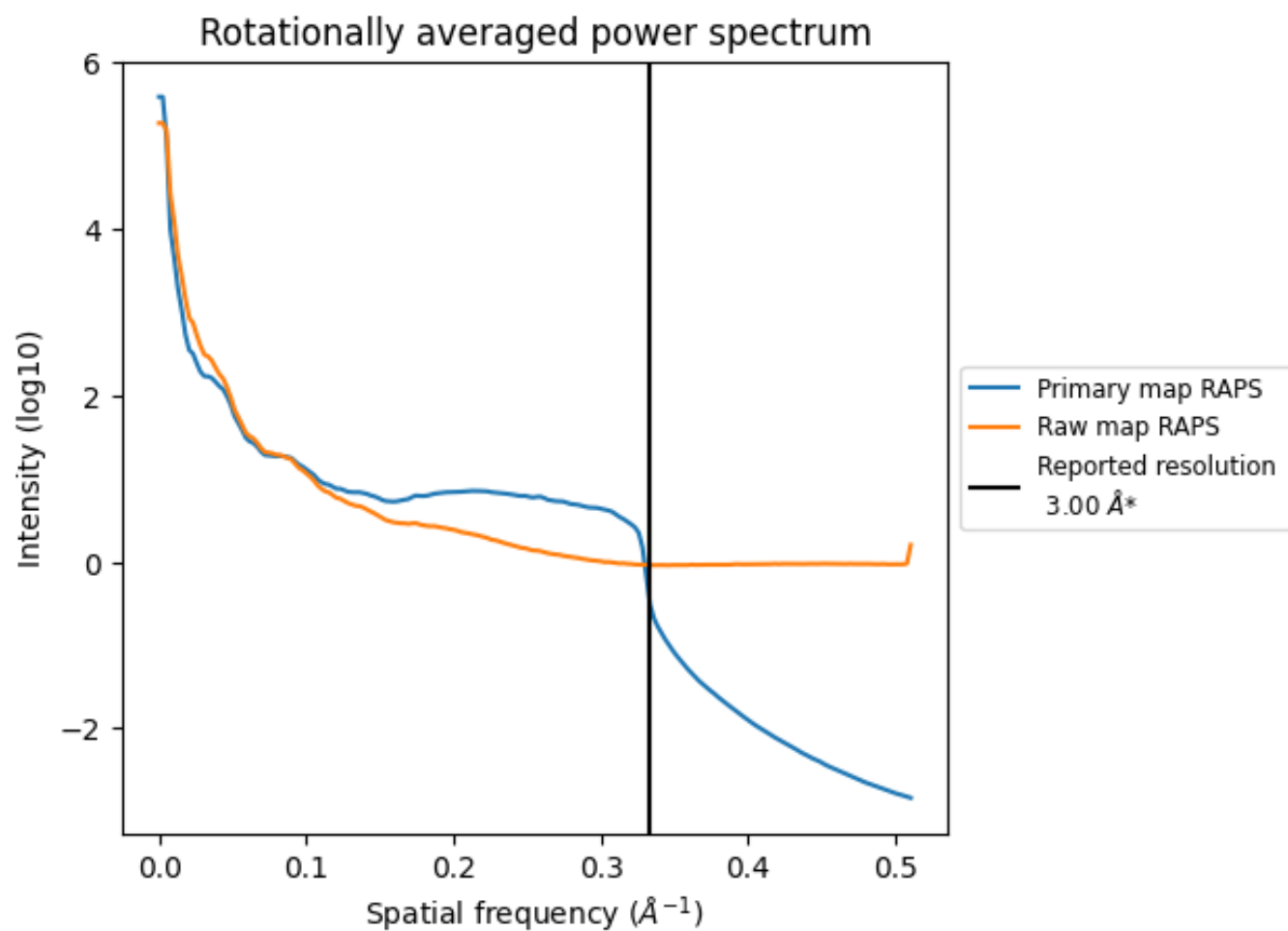
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2339 nm³; this corresponds to an approximate mass of 2113 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

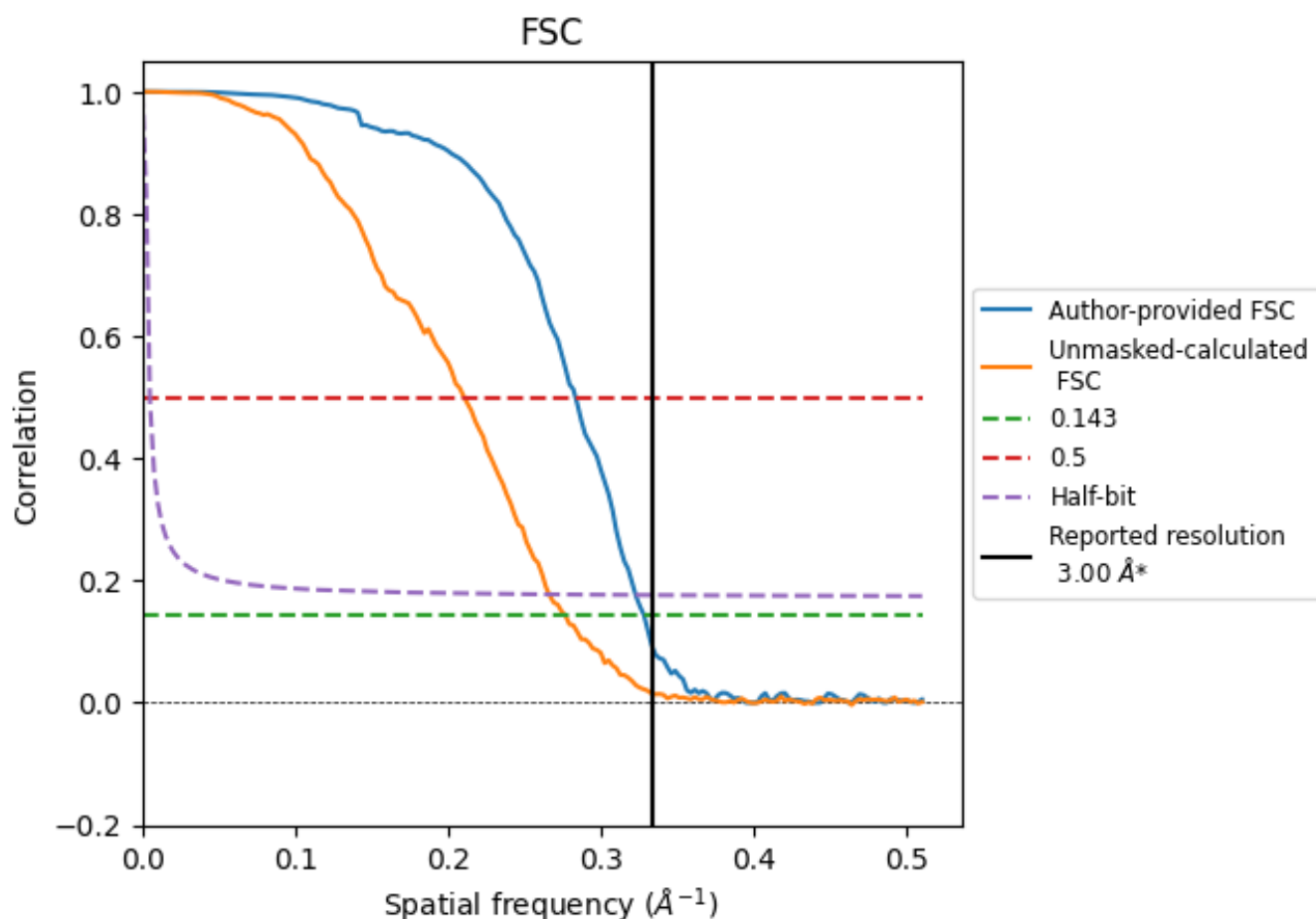


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

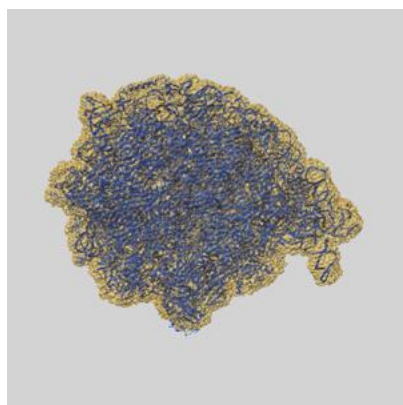
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.05	3.53	3.10
Unmasked-calculated*	3.61	4.75	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 3.0 by more than 10 %

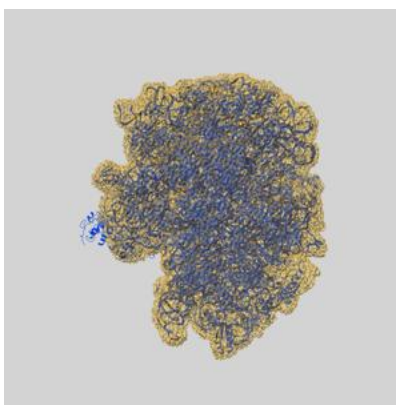
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8829 and PDB model 5WFS. Per-residue inclusion information can be found in section [3](#) on page [20](#).

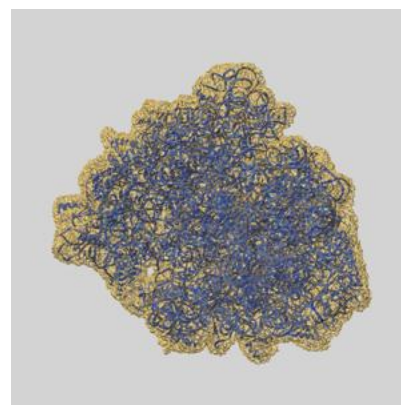
9.1 Map-model overlay [i](#)



X



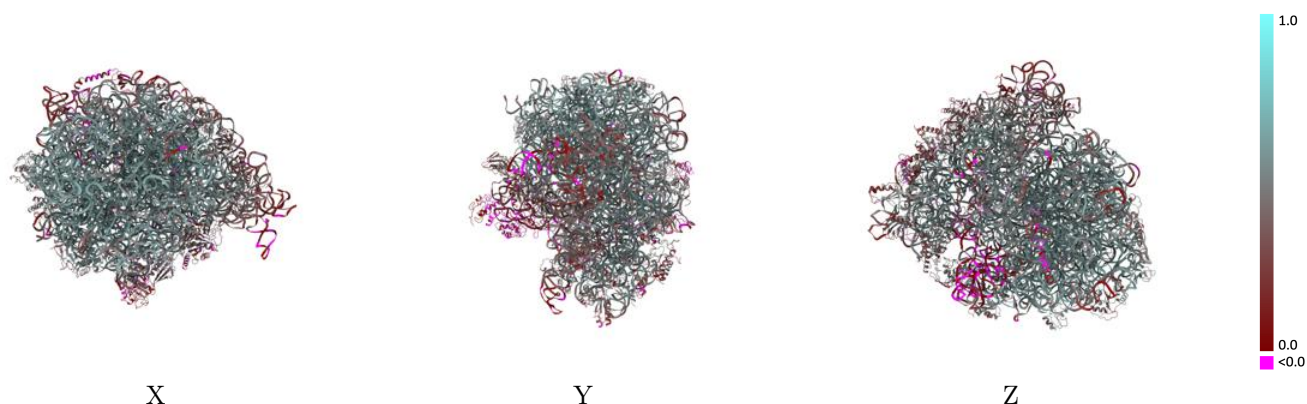
Y



Z

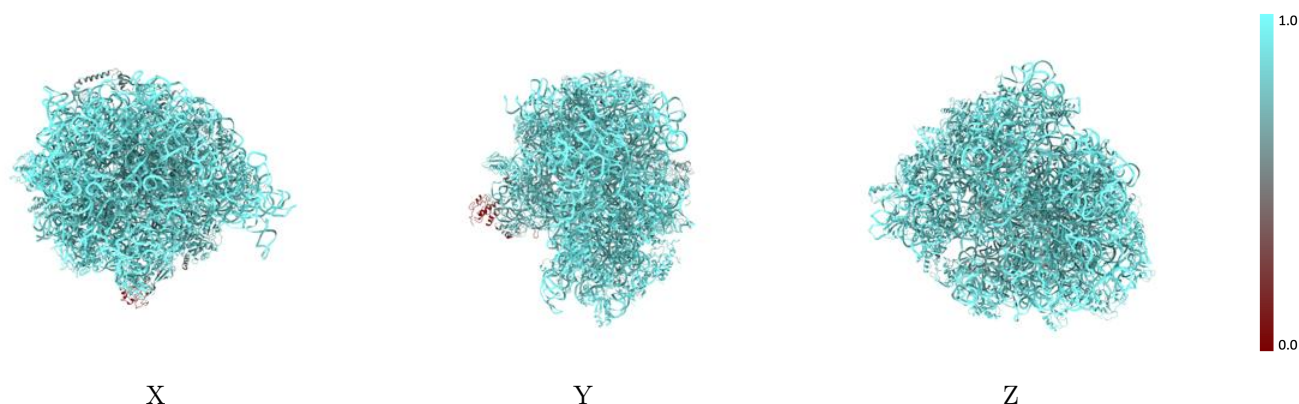
The images above show the 3D surface view of the map at the recommended contour level 0.00532 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



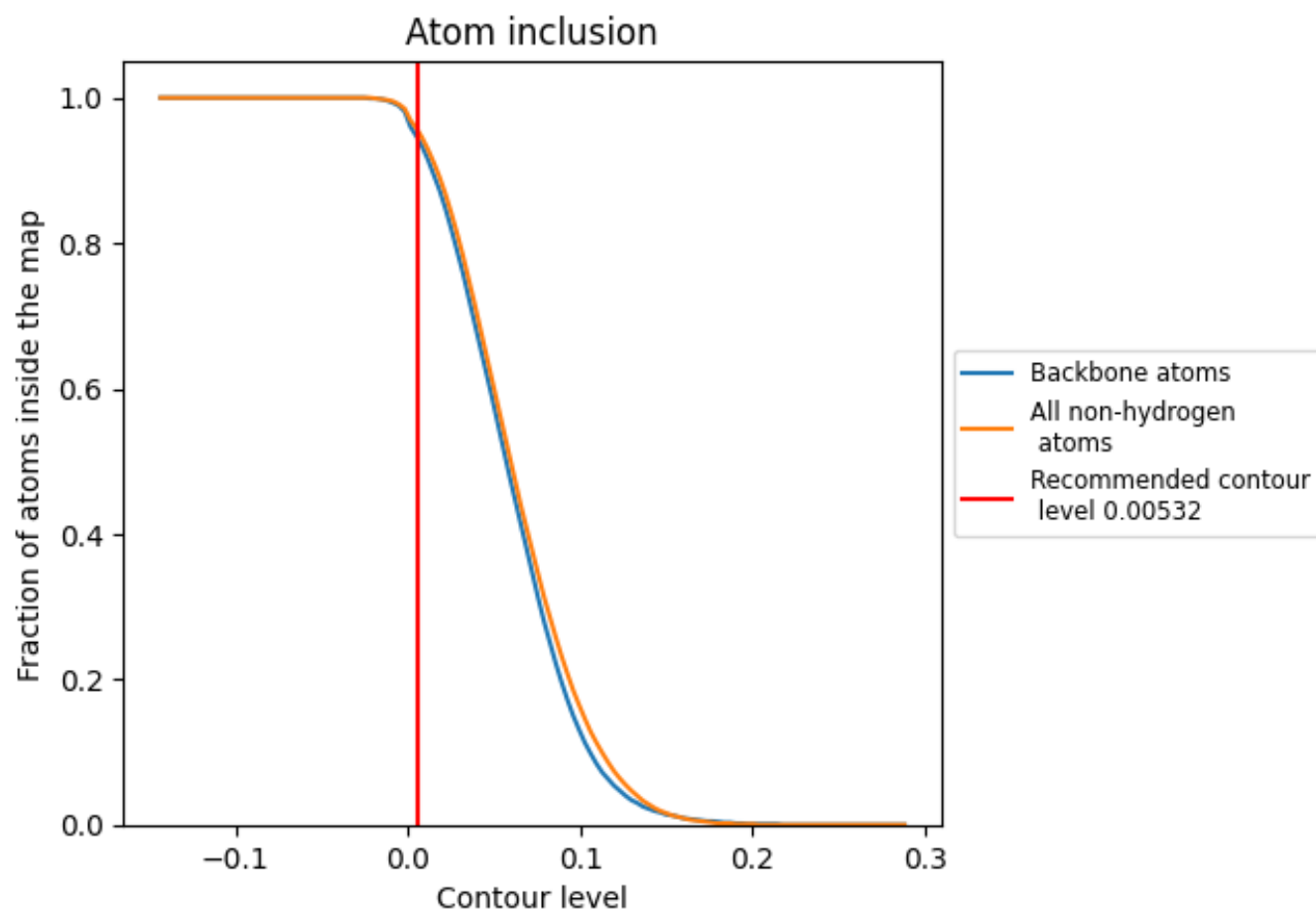
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00532).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.00532) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9570	 0.4750
0	 0.9620	 0.5080
1	 0.9240	 0.4640
2	 0.9880	 0.5860
3	 0.9840	 0.5760
4	 0.9520	 0.4940
5	 0.1120	 -0.0200
6	 0.8880	 0.3120
A	 0.9870	 0.5350
B	 0.9940	 0.5140
C	 0.9740	 0.5550
D	 0.9660	 0.5260
E	 0.9690	 0.5080
F	 0.9360	 0.4310
G	 0.9370	 0.3790
H	 0.7350	 0.2180
I	 0.6190	 0.0210
J	 0.9650	 0.5270
K	 0.9520	 0.5180
L	 0.9650	 0.5170
M	 0.9690	 0.5180
N	 0.9860	 0.5530
O	 0.9680	 0.4480
P	 0.9570	 0.5080
Q	 0.9560	 0.5500
R	 0.9390	 0.4830
S	 0.9520	 0.5230
T	 0.9340	 0.4560
U	 0.9450	 0.4450
V	 0.9490	 0.4600
W	 0.9640	 0.5480
X	 0.9550	 0.5170
Y	 0.9380	 0.4430
Z	 0.9650	 0.5020
a	 0.9870	 0.4800



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Chain	Atom inclusion	Q-score
b	 0.8950	 0.3360
c	 0.9420	 0.4360
d	 0.8990	 0.2860
e	 0.9530	 0.4820
f	 0.9230	 0.4070
g	 0.9160	 0.3700
h	 0.9490	 0.4840
i	 0.9220	 0.3850
j	 0.8960	 0.3370
k	 0.9460	 0.4300
l	 0.9080	 0.4010
m	 0.9440	 0.4280
n	 0.9500	 0.4390
o	 0.9410	 0.4440
p	 0.8930	 0.2610
q	 0.9150	 0.3710
r	 0.8970	 0.4030
s	 0.9520	 0.4260
t	 0.9200	 0.3290
u	 0.8210	 0.2580
v	 0.9720	 0.4880
w	 0.7450	 0.0740
x	 0.9840	 0.4960
y	 0.9160	 0.2870
z	 0.8290	 0.2520